Using predictive uncertainty analysis to optimise data acquisition for stream depletion and land-use change predictions

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Preface

This Master’s thesis is Antonia Margaretha op den Kelder’s degree project in Physical Geography and Quaternary Geology at the Department of Physical Geography, Stockholm University. The Master’s thesis comprises 30 credits (one term of full-time studies).

Supervisor has been Steve Lyon at the Department of Physical Geography, Stockholm University. External supervisors have been Catherine Moore and Matthew Knowling at the GNS Science in New Zealand. Examiner has been Andrew Frampton at the Department of Physical Geography, Stockholm University.

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List of Abbreviations
FOSM. First Order Second Moment
NOF. National Objectives Framework
SFR. Streamflow-Routing package
RCH. Recharge package
HK. Hydraulic Conductivity
SS. Specific Storage
SY. Specific Yield
mRECH. Recharge Multiplier
HCOND. Streambed Conductance
INCISN. Incision
ROUGHCH. Roughness coefficient
gw_level. Groundwater Level
gw_telem. Groundwater Telemetry
sw_strmflow. Surface Water Streamflow
sw_lossgain. Surface Water Loss and Gains
List of Symbols

\[ P(K|h) \] \hspace{1cm} \text{Posterior}

\[ P(K) \] \hspace{1cm} \text{Prior}

\[ P(h|K) \] \hspace{1cm} \text{Likelihood}

\[ p \] \hspace{1cm} \text{Vector containing random variables}

\[ C(p) \] \hspace{1cm} \text{Covariance matrix of random variables}

\[ h \] \hspace{1cm} \text{Observations of system state consisting of the model calibration dataset}

\[ X \] \hspace{1cm} \text{Jacobian (sensitivity) matrix}

\[ \varepsilon \] \hspace{1cm} \text{Measurement noise}

\[ s \] \hspace{1cm} \text{Prediction of interest}

\[ y \] \hspace{1cm} \text{Sensitivity of prediction of interest to model parameters}

\[ I \] \hspace{1cm} \text{Identity matrix}

\[ C(\varepsilon) \] \hspace{1cm} \text{Covariance matrix of measurement noise}

\[ \sigma^2 \] \hspace{1cm} \text{Variance}

\[ \text{DW} \] \hspace{1cm} \text{Data Worth}
Abstract

To facilitate robust understanding of the processes and properties that govern a groundwater system, managers need data. However, this often requires them to make difficult decisions about what types of data to collect and where and when to collect it in the most cost-effective manner. This is where data worth analysis, which is based on predictive uncertainty analyses, can play an important role. The ‘worth’ of data is defined here as the reduction in uncertainty of a specific prediction of interest that is achieved as a result of a given data collection strategy. With the use of data worth analysis, the optimal data types, sample locations, and sampling frequencies can be determined for a specific prediction that informs, for example, management decisions. In this study a data worth method was used to optimize data collection when predicting pumping-induced stream depletion (water quantity section) and when predicting changing nitrate concentrations as a result of land-use change (water quality section). Specifically, the First Order Second Moment (FOSM) based data worth method was employed. This thesis also builds upon previous work which explores the impacts of spatial model parameterisation on the performance of the data worth analysis in the context of stream depletion assessments. A transient groundwater model was developed, using the MODFLOW-NWT software, and a steady state transport model was developed, using the MT3D-USGS software for the mid-Mataura catchment located in Southland, New Zealand. The ‘worth’ of both existing and additional potential monitoring data were investigated. In addition, and for only the water quantity part of the thesis, three spatial hydraulic parameter density scenarios were investigated to assess of parameter simplification on the performance of the data worth method: 1) distributed pilot-point parameters. 2) homogeneous parameters, and 3) grid-cell based parameters. The water quantity (stream depletion) predictions were made at 2 key locations: (i) the catchment outlet at Gore and (ii) the outlet of a spring-fed stream (McKellar Stream). The water quality prediction (change in nitrate concentration due to land-use change) was made at 7 locations 4 key surface water locations, 2 town supply bores at Gore and one additional groundwater location further upstream. For the water quantity predictions, results show that the existing transient groundwater level data resulted in the largest reduction in uncertainty for the predictions examined. Because the low flow predictions at Gore were integrating predictions, the most uncertainty reducing observations were scattered through the catchment area with a focus on the north-west. This coincides with the recharge zone (which means that there are large water level fluctuations and hence a larger ‘signal to noise’ content in the groundwater level data). In contrast, because McKellar Stream is a discrete prediction (in this case, because McKellar Stream is spring-fed), the observations directly surrounding the stream reduce the uncertainty the most significantly. The impact of parameter simplification in the water quantity modelling showed that the data worth analysis using the grid-cell based parameterisation were very similar to those using pilot-points. However, when using the homogeneous parameterisation, the data worth results became corrupted by the lack of spatial variability available in the parameterisation. Indicating that spatial heterogeneity is needed when predicting low flows, as was shown by previous studies. However, the computational time associated with performing data worth uncertainty analyses is much higher with a grid-cell based parameterisation. A pilot-point based scheme should perhaps therefore be considered a favourable option. For the water quality predictions, results showed a strong correlation between the hydraulic conductivity, porosity and denitrification. This is likely because the hydraulic conductivity and porosity provide information about the velocity of the groundwater for a given hydraulic-head gradient, which provides information about the amount of time available for denitrification to take place in the soil substrate. Next to that, results showed no distinct difference between surface water and groundwater predictions when predicting changing nitrate concentrations, but they showed that the spatial data worth patterns depended on the proximity of the prediction location to the denitrifying areas. Overall it can be concluded that spatial parameterisation is needed when performing a data worth study for stream depletion predictions, however a more detailed parameterisation than pilot-points does not provide significantly more information. Next to that, it can be concluded that the spatial data worth patterns when predicting low flows mainly depend on if the predictions are integrating or discrete predictions. Lastly, it can also be concluded that the data worth patterns when predicting change in nitrate concentration depend on the proximity of the prediction location to the denitrifying areas.
1. Introduction

1.1 Motivation
Effective conjunctive management of surface water and groundwater resources requires that a robust understanding of the system under investigation exists. This includes a good understanding of the potential impact of groundwater abstraction and land-use changes on surface waters (both in terms of quantity and quality). Assessment of such impacts, e.g., pumping-induced stream depletion, surface water quality degradation following e.g. dairy-farm intensification, are commonly undertaken as a means of informing freshwater allocation limit-setting policy (e.g., Tim et al., 1994; Letcher et al., 2004; Schlüter et al., 2005).

To facilitate robust understanding of groundwater and the processes and properties that govern groundwater systems, managers need to make difficult decisions about what types of data to collect and where and when to collect them. Monitoring is expensive and time consuming, therefore it is important that the most meaningful data, for the lowest cost, are obtained. This is where data worth analysis, which uses predictive uncertainty analyses, can play an important role. With the use of data worth analysis, the optimal data types and their sample locations and sampling frequency can be determined for a specific prediction (Wallis et al., 2014). This thesis will use the data worth method to optimize data collection for both water quality and quantity predictions, and specifically it employs the First Order Second Moment (FOSM) based data worth method (Kikuchi, 2017).

A number of recent papers in the literature have employed numerical models and the FOSM version of data worth method, as a means of assessing data worth. For example, Dausman et al. (2010) explored the worth of temperature and salinity observation for predictions related to the movement of the freshwater salt-water interface in reaction to a reduction in the recharge of freshwater. They used a hypothetical salt and heat transport model and found that concentration measurements reduced the initial uncertainty the most, and thus were the most valuable. Fienen et al. (2010) demonstrated the use of the data worth method when designing a monitoring network, next to that they address the importance of a distributed spatial parameterisation when using the data worth method. Wallis et al. (2014) used the data worth method to explore which combination of tracers used in injection tests (methane, temperature, chloride, and bromide) are the most cost-effective. They concluded that even though temperature data were the least-informative they were still recommended because of the low costs of acquiring the data.

Although there are an increasing number of studies that have used the data worth method, this thesis focuses on the application of the method in four new ways. Firstly, the study compares the relative worth of the hydraulic heads, stream flow and surface water-groundwater exchange observations in both space and time in the context of stream depletion forecasting. Additionally, this thesis builds upon the work by Fienen et al. (2010), by exploring the impacts of spatial parameterisation on the performance of the data worth analysis in the context of stream depletion assessments. Thirdly, this study explores the interplay between existing and new observations on the data worth analysis output. Fourthly, this study explores the worth of groundwater and surface water nitrate concentration observations for the predictions concerning nitrate concentration changes as a result of land-use changes.

1.2 Background
The data worth methodology uses four main components, a physically based numerical model, a model prediction, the sensitivity of the prediction to model parameters, and a description of parameter and measurement uncertainties. The model predictions provide the focus of the data worth analysis, e.g. the worth of any data is defined in terms of the extent to which the uncertainty of that prediction is reduced by the information furnished by the data. The theory behind and the mathematical basis of the data worth equation is described in chapter 3. Uncertainty Analysis: Theoretical Background. Two groups of predictions are used to focus the data worth analysis undertaken in this study, one group focussing
on the stream depletion assessment and one on the land use change impacts on water quality assessment as are now described.

Surface water low-flow characteristics are widely used by decision-makers as a basis for devising water-use allocations (e.g., Fisher et al. 2009) and maintaining aquatic health (e.g., Maddock, 1999). Transient flow variability can be conceptualised using flow duration curves. The flow duration curve plots the discharge against the percentage of time exceedance (Cigizoglu & Bayazit, 2000). The flow duration curve allows for the quantification of low-flows using the Q95. The Q95 means that in 95% of the time the flow is higher than the discharge at that point (Werritty, 2002). Figure 1.1 shows a schematic representation of a flow duration curve and the Q95.

One part of this study is to investigate the worth of monitoring data (data type, monitoring locations and monitoring frequency) in the context of predicting the amount of days, and the amount of consecutive days, below Q95, the grey area in Figure 1.1. The Q95 is closely related to the amount of discharge below which aquatic animals become stressed (Dunbar et al., 2010). An increase in amount of days below Q95, e.g., in response to groundwater abstraction, would therefore have large ecological implications.

![Flow Duration Curve (FDC) and Q95](image)

The second part of this study will investigate what type of observation data and monitoring locations will be the most valuable when looking at changing nitrate concentrations in both the groundwater and surface water as a result of land-use changes.

Animal excrements and the use of (artificial) fertilisers and imported feed have been shown in the literature to cause elevated nutrient (nitrogen and phosphorus) levels in both soil and groundwater (Di & Cameron, 2002; Wang et al., 1999). The presence of excess nutrients is related to a variety of environmental problems. One large environmental implication of excess nutrients is that it can lead to eutrophication. Eutrophication happens when a large amount of nutrients is added to a water body. Due to the enrichment in nutrients, excessive growth of algae and plants take place, which often leads to an increase in periphyton biomass. This is also referred to as an algal bloom. As a consequence, the amount of oxygen in the water decreases. This can result in the death of fish and other aquatic animals, ultimately decreasing the biodiversity of the system (Smith et al., 1999).

As well as eutrophication, nitrogen can also cause health problems. In the soil, nitrogen is converted into nitrates and nitrites through a process called nitrification (Skinner et al., 2000). Nitrate is regarded as a regulated drinking water pollutant and can have a variety of negative health impacts if consumed...
Due to these effects, it is crucial that the amount of nitrate in surface- and groundwater is effectively monitored and managed.

1.3 Aim of the Study and Experiment Overview
This study consists of several components, this is presented in the flow chart in Figure 1.2. The study can be roughly divided into two sections: 1) Water quantity and 2) Water quality.

Three predictions, are investigated in section 1) Water quantity:

1) the difference in the amount of days below Q95 between the original model and a model with additional pumping wells.
2) the difference in the amount of consecutive days below Q95 between the original model and a model with additional pumping wells.
3) the difference in discharge between the original model and a model with additional pumping wells (magnitude of stream depletion).

These three predictions are investigated for two locations. The worth of the existing data is investigated as well as which additional data and where would be the most valuable for the different predictions for both locations.

The effects of simplification are explored for the number of days below Q95 and the magnitude of stream depletion predictions. The analyses are repeated for both a simpler and a more complex model parameterisation. Three spatial hydraulic parameter density scenarios were investigated: 1) distributed pilot-point parameters, 2) homogeneous parameters, and 3) grid-cell based parameters.

In section 2) Water quality, one prediction is investigated:

4) the difference in predicted nitrate concentration between the original transport model and a model with double the initial nitrate concentration.

This prediction is investigated at seven locations: four surface water concentration locations, and three groundwater concentration locations. For all these locations, the worth of both existing and additional data is investigated.

In short, this thesis aims to determine which type and location of data are the most valuable for the predictions described above, and to identify the effects of model parameterisation simplification on the results. In order to do so, the following research questions are addressed:

Water Quantity questions:
- How well are the flow model parameters informed by the existing data? What is the role of parameters in uncertainty?
- How valuable is the existing data, and which type of additional data, collected where and when, will be the most valuable when predicting the number of days, and number of consecutive days, below a specified low stream flow rate (e.g. a Q95 flow rate), and what the pumping induced stream depletion rate?
- How do the spatial data worth patterns differ when the predicting impacts at different locations e.g. at Gore and McKellar Stream?
- For the predictions of the number of days below the Q95 flow rate and the magnitude of stream depletion rate: how is the reduction in uncertainty impacted when having a less dense monitoring network? How is the reduction in uncertainty impacted when decreasing the monitoring frequency?
- Are the data worth analysis results for the water quantity predictions impacted by model parameterisation simplifications? How are the final results impacted if a model uses a homogeneous, pilot-point, or grid-cell based parameterisation?
Water Quality questions:
- What is the role of the parameters in the uncertainty surrounding water quality predictions?
- How valuable is the existing data, and which type of data, collected at which location, will be the most valuable when predicting the change in nitrate concentration resulting from land use change? Is there a difference in the data worth results between the groundwater and surface water nitrate predictions?

The study will be performed in the form of a case study on the mid-Mataura river catchment.

Figure 1.2. Flow chart of the different layers of this master thesis. A) Water Quantity section, the overarching layer is model simplification. The goal is to investigate the effects of using a homogeneous, pilot-point, and grid-cell based model parameter distribution. Three predictions are investigated for two locations and for all of them the worth of the existing data and which type of additional data and where would be the most valuable is investigated. B) Water Quality section, one prediction for seven locations (three groundwater concentrations and four surface water concentrations). For all these locations data worth is calculated for the existing and additional new data.

This thesis consists of 7 chapters, including this introductory chapter. The study area is described in chapter 2. Chapter 3 is about the theory behind the predictive uncertainty analysis. Chapter 4 describes the data and methodology that are used. The results are presented in chapter 5 and discussed in chapter 6. Finally, in chapter 7 the study is summarized and the conclusions are presented.
2. Regional Settings

2.1 General Description
This study focusses on the upper section of the mid-Mataura catchment, located in Southland on New Zealand’s South Island (Figure 2.1). Southland is both the most westerly and southerly part of New Zealand (Macara, 2013). The study area is located in the north-western part of Southland, with the Southern Alps to the west. The location of the Southern Alps has a large impact on the overall climate of the study area. The study area is relatively flat and surrounded by mountainous areas. There is a difference in relief of approximately 150 m asl to 80 m asl at Gore. The study area is surrounded by the Hokonui hill ranges in the South and the Mataura ranges in the North (“Mid-Mataura Groundwater Model”, 2007).

Figure 2.1, Geological map of the study area with the catchment of the mid-Mataura river outlined in red. The yellow colours indicate Quaternary deposits (Turnbull & Allibone, 2003).

The mid-Mataura catchment is one of the largest catchments in New Zealand, and has great recreational and economical value (Wilson, 2008; Wilson, 2010). The catchment has been impacted by human activity for a long time. Between 1940 and 1980 widespread alterations to the catchment have taken place: clearing of land, straightening of channels, and the installation of artificial drainage systems. In addition, more than 70 percent of the land has been altered to make it suitable for farming. In order to protect the water quality and quantity the Acclimatisation Societies applied in 1984 for a National Water Conservation Order (Riddell, 1984). The Water Conservation (Mataura River) Order was implemented in 1997. In the Water Conversation Order, minimum water quality requirements were set, and a maximum water allocation amount was described. The threshold for water allocation was set to five percent of the natural flow in the Mataura rivers (Wilson, 2010). Groundwater demand in Southland has increased dramatically, mainly because of an increase in irrigation (Wilson, 2008). Because of this large change in water usage it is important to know the impacts of that on the streamflow.
In addition to the changes in water quantity usage in the mid-Mataura catchment, significant land use changes have taken place. The area was traditionally used for beef, sheep, and arable farming. But there has since been a general shift to dairy farming (Wilson, 2010; Lilburne et al., 2012). Figure 2.2 shows the amount of livestock in the Southland region for the period 1860-2010. It is clear that there has recently been an increase in dairy stock. These land-use changes have significantly impacted the amount of nitrate loading in the mid-Mataura catchment. Figure 2.3 shows the amount of nitrate loading in the catchment area in kg/d/ha for A) 1996 and B) 2015. It is clear that the amount of loading has significantly increased over time.

Four different periphyton biomass objectives have been specified by the National Objectives Framework (NOF). Each biomass objective has a specific nutrient threshold (e.g. phosphorus and nitrogen) that are not be exceeded to ensure the biomass objectives are achieved (Snelder et al., 2013). It is critical to understand and reliably estimate surface water nitrate concentrations, to be able to investigate if the NOF-specified thresholds will be exceeded.
Previous model studies have been performed for the mid-Mataura catchment. In 2007 a hydrogeological model, commissioned by Environment Southland, was developed to assess the impacts of groundwater abstraction. The model showed that the extraction of groundwater already had an impact on the discharge (“Mid-Mataura Groundwater Model”, 2007). Since this model is over 10 years old, and our process understanding and modelling capabilities have likely improved, as such a new model for the mid-Mataura catchment was developed by GNS Science. This new model will be used as the foundation of this study. To date, no data worth study has been performed in the area.

2.2 Physiographic Zones
The regional council for the area, Environment Southland, currently has a project called Water and Land 2020 & Beyond. Part of this project was to divide Southland in different physiographic zones that will help with managing water quality and the effects of land use changes. The physiographic zones are based on a variety of factors, such as geology, topography, soil type, and climate. In total nine different physiographic zones are identified for the Southland region. The study area is diverse, seven of the physiographic zones are present in the catchment (Figure 2.4). These seven are described in Table 2.1. Each zone differs in how contaminant accumulate and are transported through the soil and groundwater system into the rivers and streams. (Rissmann et al.; Snelder et al., 2016). One of the most important differences between the physiographic zones is the dominant contaminant pathway(s) (Table 2.1). The physiographic zones are not directly used in this study, but they do give a good impression of the study area composition.

Figure 2.4. Map with the different physiographic zones present in the study area. The mid-Mataura catchment is outlined in red, blue lines indicate streams (Data: ESR (pers. comm. 2017)).
### Table 2.1. The different physiographic zones that are present in the study area along with their dominant contaminant pathways and a general description (Snelder et al. 2016).

<table>
<thead>
<tr>
<th>Physiographic Zone</th>
<th>Dominant Contaminant Pathways(s)</th>
<th>General description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bedrock/Hill Country</td>
<td>Artificial drainage, overland flow, lateral flow</td>
<td>Located below 800 m asl. Glacial till or bedrock found near the surface. Large areas of groundwater are absent.</td>
</tr>
<tr>
<td>Gleyed</td>
<td>Artificial drainage</td>
<td>Poorly drained soils in low-lying areas. The occurrence of waterlogging is common. Denitrification in the soils and aquifer takes place.</td>
</tr>
<tr>
<td>Lignite/Marine Terraces</td>
<td>Overland flow, deep drainage, artificial drainage</td>
<td>Contains soils with a high organic matter content. The water quality in this zone is strongly influenced by geology.</td>
</tr>
<tr>
<td>Old Mataura</td>
<td>Deep drainage</td>
<td>In general, the soils are highly weathered, well drained, and tend to accumulate nitrogen. Nitrogen levels in groundwater can reach high levels.</td>
</tr>
<tr>
<td>Oxidising</td>
<td>Artificial drainage, overland flow, deep drainage</td>
<td>Soil and groundwater have very high levels of oxygen and low denitrification potential. As a consequence, nitrogen tends to accumulate in these soils.</td>
</tr>
<tr>
<td>Peat Wetlands</td>
<td>Lateral flow, artificial drainage</td>
<td>Low lying flat land. High organic matter content and high denitrification ability causes low amount of nitrogen accumulation</td>
</tr>
<tr>
<td>Riverine</td>
<td>Deep drainage</td>
<td>Areas next to the main rivers and streams. It also includes the floodplains and low elevation terraces.</td>
</tr>
</tbody>
</table>

#### 2.3 Hydrogeology and Aquifer Properties

The subsurface for the main aquifer unit consists of late Quaternary and Holocene fluvial terrace deposits. The sediments mainly consist of poorly sorted gravels, sand, and silt. Underneath these sediments are Tertiary sediments with low permeabilities. The start of this low permeability layer is also regarded to as a ‘groundwater basement’ and is used to define the bottom of the aquifer (“Mid-Mataura Groundwater Model”, 2007).

The Mataura river gains flow from aquifer drainage, particularly towards the bottom of the catchment, where almost all the groundwater discharges into the river. Because of this, during extended periods of no rainfall the low flow in the river represents the constant head of the groundwater (“Mid-Mataura Groundwater Model”, 2007).

An important property of the subsurface, in terms of this study, is its ability for denitrification. Denitrification will take place in the subsurface if there is no oxygen present (Fetter et al., 2017). Figure 2.5 shows the study area and it is divided into three types: oxidised, mixed, and reduced. Oxidised means that there is oxygen present and thus there will be no denitrification. Reduced means that there is little to no oxygen present and that denitrification will take place. The mixed zone is a bit of both, denitrification could take place here, but it is not a certainty. The spatial occurrence of denitrification in the transport model is based on the zones in Figure 2.5.
2.4 Climate

According to the Köppen-Geiger climate classification, the mid-Mataura catchment lies in a temperate zone and has a maritime climate (Cfb) (Kottek et al., 2006). The climate, and especially rainfall, is highly variable throughout Southland (Macara, 2013). Figure 2.6 shows the median total rainfall for the Southland region for the period 1981-2010. The figure clearly shows that there is a strong orographic rain shadow effect in the region caused by the southern part of the Southern Alps (Ledgard, 2013). In the mountain ranges the total annual rainfall can be more than 6000 mm, but because of this orographic effect, the total annual rainfall in the study area is between 800 and 1000 mm (Figure 2.6) (“Mid-Mataura Groundwater Model”, 2007).

Figure 2.7 shows the average annual temperature and the average total monthly precipitation for the period 1987-2017 for the weather station located in Gore, which is situated at the bottom of the catchment. This figure shows that the climate is very temperate, with the temperature ranging from approximately 5 °C in winter to approximately 15 °C in summer. Rainfall occurs all throughout the year and a clear dry period is absent. The total monthly rainfall is slightly lower during the winter months July and August compared to the summer months December and January, this coincides with the period when low flows generally occur.
Figure 2.6. The median annual total rainfall for the Southland region for the period 1981-2010 (Macara, 2013).

Figure 2.7. Average monthly temperature (°C) and total monthly precipitation (mm). The values are averaged for the period 1987-2017 for the station GoreAws, lat: -46.115, long: 168.887 (Data: National Institute of Water and Atmospheric Research (NIWA)).
3. Uncertainty Analysis: Theoretical Background

Uncertainty is inherent in models due to the imperfect knowledge of the parameters and the system in general. The quantification of predictive uncertainty is increasingly common in groundwater modelling practice (Doherty, 2015). Uncertainty quantification provides a platform for risk-based model usage, which as Doherty and Simmons (2013) point out constitutes the only way in which model-based decision-making should be carried out.

Uncertainty and probability are related quantities, with probabilities essentially providing a quantification of uncertainty. Probability can be defined as the likelihood that a specific event will happen (Doherty, 2015). The probability of an event can be expressed using a probability density function (pdf). The most commonly used pdf, which is also assumed in this study, is the Gaussian or Normal distribution. The normal distribution has a characteristic bell-shaped curve (Doherty, 2015). Figure 3.1 shows an example of a normal distribution. In black is shown the original pdf. In red is shown how the pdf will look after a reduction in uncertainty. The area underneath the graph will remain the same, but the width of the pdf will be decreased.

Figure 3.1, Normal or Gaussian distribution. In black an example of a pdf, in red an example of the same pdf after a reduction in uncertainty (Adapted from Doherty, 2015).

3.1 Uncertainty Analysis Methods

A variety of methods can be employed to perform uncertainty analyses. The two main types of methods are global and local, and both have their roots within Bayes’ theorem.

3.1.1 Bayes’ Equation

Bayes’ theorem states that available information updates the pdf. Bayes equation is displayed in eq. 3.1, in terms of groundwater modelling the $K$ stands for parameter and $h$ for observation. According to Bayes’ theorem, the pdf, also called posterior ($P(K|h)$), is proportional to the prior pdf ($P(K)$) times the likelihood ($P(h|K)$) (Bayes, 1763).

$$P(K|h) \propto P(K) \times P(h|K)$$  \hspace{1cm} eq. 3.1

In this case the prior pdf could be all the possible values a certain parameter could have, and reflects our “expert knowledge” of system parameters. The likelihood component would incorporate the possible values that the parameter could have according to observational data. Multiplying these two components results in the posterior pdf (Dausman et al., 2010).

3.1.2 Global Uncertainty Analysis Methods

Global uncertainty analysis methods are a ‘purer’ application of the Bayes’ theorem (Doherty, 2015; Rawlinson et al., 2018). Global methods are computationally much more intensive than the local methods because they explore multi-dimensional parameter space. The main thing global methods rely on is the quantification of uncertainty through random sampling (e.g., Monte Carlo) (Rawlinson et al., 2018).
One example of the global uncertainty analysis methods is called “rejection sampling”. In this method, the model is run numerous (usually many) times until the model fits the observation data. This is computational very intensive and not suitable for models with long run times, which is often the case for groundwater modelling (Rawlinson et al., 2018).

3.1.3 Local Uncertainty Analysis Methods

Local uncertainty analysis methods are more simplified than the global uncertainty analysis methods. A large assumption that is made in local methods is that the model that is used is linear (i.e., the relationship between model outputs and parameters is constant across parameter space). As a result, it is computational much less intensive, but it should be noted that because of that assumption the results are an approximation (Morio, 2011; Rawlinson et al., 2018). The local methods are also referred to as ‘error propagation methods’ or First Order Second Moment (FOSM). The FOSM method approximates the first order derivatives using a Jacobian matrix. The goal of FOSM is to calculate the variance of a calculated output based on the variance of the input terms. This is the basis of the data worth method described below in section 3.4 Data Worth Method.

Let \( p \) be a vector of random variables that can be split into two subvectors \( p_1 \) and \( p_2 \):

\[
\mathbf{p} = \begin{bmatrix} \mathbf{p}_1 \\ \mathbf{p}_2 \end{bmatrix}
\]  
\text{eq. 3.2}

As a result, the covariance matrix of \( \mathbf{p} \), \( \mathbf{C}(\mathbf{p}) \), is given by:

\[
\mathbf{C}(\mathbf{p}) = \begin{bmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{bmatrix}
\]  
\text{eq. 3.3}

The covariance matrix comprises of variances on the diagonal and the parameter covariance on the off-diagonal sides. When the components of \( \mathbf{p}_2 \) become known (i.e., when \( C_{22} \) equals zero), the conditional covariance matrix of \( \mathbf{p}_1 \), \( \mathbf{C}'_{11} \), can be calculated as shown in eq. 3.4 via the Schur Complement (the second term of the right-hand side of eq. 3.4) (Koch, 1987).

\[
\mathbf{C}'_{11} = C_{11} - C_{12} C_{22}^{-1} C_{21}
\]  
\text{eq. 3.4}

Eq. 3.4 can be used to define the reduction in uncertainty of model parameters (and subsequently the predictions that depend on these parameters) (Dausman et al., 2010). This is accomplished by considering the role of additional data that consists of information that is relevant to the model parameters in reducing parameter uncertainty (Dausman et al., 2010; Wallis et al., 2014).

Let \( \mathbf{p} \) consist of the values of parameters used by a model. Also, let the matrix \( \mathbf{X} \) represent the (linear) relationship between model outputs and model parameters. The matrix \( \mathbf{X} \) is also referred to as the Jacobian (or sensitivity) matrix. In order to fill a Jacobian matrix, the model has to be run as many times as there are parameters, plus one additional time to establish a “base” condition against which derivatives are calculated. If elements of the Jacobian matrix are large, it means that those observations are sensitive to parameters. The vector \( \mathbf{h} \) stands for the observations of system state consisting of the model calibration dataset. And finally, the vector \( \mathbf{e} \) contains the measurement noise associated with these observations and the structural (epistemic) noise (Dausman et al., 2010; Wallis et al., 2014). The relationship between model inputs, outputs and observations is displayed in eq. 3.5.

\[
\mathbf{h} = \mathbf{Xp} + \mathbf{e}
\]  
\text{eq. 3.5}

Let \( s \), which is a scalar, stand for the prediction of interest made by the model. The sensitivity of this prediction to model parameters is characterized by the vector \( \mathbf{y} \) (Dausman et al., 2010; Wallis et al., 2014). Eq. 3.6 shows how \( s \) can be calculated.

\[
s = \mathbf{y}^t \mathbf{p}
\]  
\text{eq. 3.6}
Combining eq. 3.5 and eq. 3.6 gives:

\[
\begin{bmatrix}
    s \\
    h
\end{bmatrix} =
\begin{bmatrix}
    y^t \\
    X
\end{bmatrix}
\begin{bmatrix}
    0 \\
    1
\end{bmatrix}
\begin{bmatrix}
    p \\
    \varepsilon
\end{bmatrix}
\]

Eq. 3.8 shows how the covariance matrix of \(s\) and \(h\) is calculated. This formula is the result when the standard matrix relationship for propagation of covariance is used (Dausman et al., 2010; Wallis et al., 2014).

\[
C\left(\begin{bmatrix} s \\ h \end{bmatrix}\right) =
\begin{bmatrix}
    y^t \\
    X
\end{bmatrix}
\begin{bmatrix}
    0 \\
    1
\end{bmatrix}
\begin{bmatrix}
    C(p) & 0 \\
    0 & C(\varepsilon)
\end{bmatrix}
\begin{bmatrix}
    y \\
    X^t
\end{bmatrix}
\]

\[
= \begin{bmatrix}
    y^tC(p)y & y^tC(p)X^t \\
    XC(p)y & XC(p)X^t + C(\varepsilon)
\end{bmatrix}
\]

In eq. 3.8, \(C(p)\) stands for the covariance of parameter uncertainty, the identity matrix is represented with \(I\), and the \(C(\varepsilon)\) stands for the covariance matrix of the measurement and structural noise (Dausman et al., 2010; Wallis et al., 2014). When eq. 3.4 is applied to eq. 3.8 it gives eq. 3.9.

\[
\sigma_s^2 = y^tC(p)y - y^tC(p)X^t[XC(p)X^t + C(\varepsilon)]^{-1}XC(p)y
\]

Where \(\sigma_s^2\) is the predictive uncertainty variance of prediction \(s\). The first term on the right \((y^t C(p)y)\) represents the “prior” uncertainty of a prediction, i.e., before observations are acquired. Note this term is analogous to the \(P(K)\) term in Bayes’ theorem (eq. 3.1). The second term on the right represents how much the prior predictive uncertainty will be reduced by this constraining effect of observations (Dausman et al., 2010; Wallis et al., 2014). Note this term is analogous to the \(P(h|K)\) term in Bayes’ theorem (eq. 3.1).

### 3.2 Regularization

Fienen et al. (2010) show that for some predictions a highly-parameterised model is needed in order to achieve reliable data worth analysis. They showed that the results when using a pilot-point based hydraulic conductivity distribution gave much better results than when using large zones of uniform values. All highly parameterised models are ill posed (i.e. there are more unknowns (model parameters) than equations (observations)). There is therefore no (unique) solution as model output (Tikhonov & Arsenin, 1977). Ill-posed problems require regularization. Regularization can be performed by introducing additional “observations” (e.g., in the form of prior information on parameters) such that the inverse problem becomes mathematically tractable or “well-posed” (Engl et al., 1996). This form of regularization is referred to as Tikhonov regularization (Tikhonov & Arsenin, 1977).

It can also be performed by parameter reduction techniques such as Singular Value Decomposition or through Tikhonov regularization. A combination of both can also be used (Doherty, 2015). While regularization is not directly used in the data worth method, it does play an important role during the calibration process of highly parameterised models, as used in this study.

### 3.3 Simplification

As said above, models are used to learn more about the natural systems and in order to predict what effects certain changes could have on the natural system. As a consequence, an attempt is made to make models as close to reality as possible. This leads to highly complicated models which are computationally intensive and have long run times. Doherty and Moore (2017) argue that there should be a shift from trying to make a highly-complicated model that can, theoretically, be used for all predictions, to using models in a more direct and targeted way to test whether a hypothesis can be rejected. This reverses the modelling process: now a model will be built towards making a specific prediction and will thus not need all the complexities of the real world. Doherty and Simmons (2013) point out that, when adopting this new modelling strategy, a false region of a hypothesis (i.e. type-II
statistical error) should be avoided; this constitutes failure of a model to do its job. In other words, a model should be designed to be complex enough to avoid such a false hypothesis rejection. This can be done by making sure that there is an overestimation of the uncertainty of the prediction. One aspect of this study is to see what the impacts of model simplification in terms of parameterisation will have in terms of uncertainty quantification and data worth analyses.

3.4 Data Worth Method

Data worth analyses are often based on the principle that the worth is related to the reduction in uncertainty of a specific prediction of interest as a result of data collection (e.g., Moore and Doherty, 2005; Christensen & Doherty, 2008; Wallis et al., 2014). In other words, a new observation will have a high worth if it reduces the uncertainty of a prediction significantly, and the worth of a new observation will be low if there is minimum to no change in the original uncertainty of the prediction. In this thesis, the FOSM based data worth method is used (as referred to in Kikuchi, 2017). The non-FOSM based data worth methods (as described above) are not suitable to use in this study because they are much more computationally intensive and as a result they would take too long and hence are not a pragmatic choice.

In order to quantify “data worth” eq. 3.10 is used.

\[ DW = \left( 1 - \frac{\sigma_{+\text{obs}}^2}{\sigma_{\text{base}}^2} \right) \times 100 \]  

_eq. 3.10_

Eq. 3.10 shows that data worth (DW) is quantified as the percent decrease in the predictive uncertainty variance when a new observation is made. In this equation \( \sigma_{\text{base}}^2 \) is the predictive uncertainty prior to the addition of one or a group of new observations, and \( \sigma_{+\text{obs}}^2 \) is the predictive uncertainty when the new observation or observations are added (Fienen et al., 2010; White et al., 2016). If the DW percentage is high, it indicates that the new observation decreased the initial uncertainty significantly, i.e., the additional data is of significant worth. Alternatively, the method can be used to quantify the increase in predictive uncertainty incurred by the omission of certain types of data from the calibration dataset, and therefore be employed to explore the cost in increased predictive uncertainty incurred by ignoring information that is contained in historical transient groundwater behaviour.

For a more detailed description and derivation of the equations, see Christensen & Doherty (2008) and Fienen et al. (2010).
4. Data and Methodology

4.1 Water Quantity

4.1.1 Groundwater Flow Model

The groundwater flow model used in this study has been developed by GNS Science. The model simulates transient groundwater flow conditions using the MODFLOW-NWT (Niswonger et al., 2011) software. MODFLOW-NWT was selected because of its enhanced ability to handle cell drying and (re-) wetting non-linearities (Niswonger et al., 2011). The model simulates groundwater flow for an unconfined aquifer at a daily temporal resolution. The model domain extent was based on previous studies and re-examination of the catchment boundaries (“Mid-Mataura Groundwater Model”, 2007). It is a 1-layer model that has 180 rows and 176 columns, each cell is 250 m by 250 m. The model simulates flow spanning the period from 2000-01-01 until 2015-01-02. The study is performed on the uncalibrated version of the model. There are 150 extraction wells present in the model (Figure 4.1). The initial model setup was configured using the graphical user interface GMS. After that the MODFLOW packages were altered using a text editor and Python package FloPy.

![Figure 4.1. Spatial distribution of the extraction wells present in the catchment. Wells are indicated with black dots. Model domain extent is shown in red and the blue lines indicate the streams.](image)

The catchment is essentially an enclosed basin, which means that there is no significant groundwater exchange between inside and outside the model domain. In order to simulate the streams and the surface water and groundwater exchange in the model the Streamflow-Routing (SFR) package is used. The SFR package contains a constant influx of discharge based on model outputs from the TopNet model (Clark et al., 2008) provided by NIWA. The Recharge (RCH) package provides influx into the model based on precipitation data.

Initial conditions were set for the hydraulic head. This was achieved by running the groundwater flow model twice, to ensure that the head values had stabilised at a level commensurate with the observed heads at the beginning of the model simulation period (i.e. there were no sudden rises or drops in head between the initial conditions and the first simulation stress period).

The uncertainty associated with spatially distributed hydraulic conductivity (HK), specific storage (SS), specific yield (SY), and recharge multiplier (mRECH) parameters are considered in this study. Spatial variability in these parameters are parameterised using pilot-points. In total, there are 350 pilot-points per different parameter type, each pilot-point separated by 2 km. The model solves for each pilot-point and then interpolates remaining model grid values using a kriging interpolation method based on a semivariogram (Zimmerman et al., 1998). The semivariograms used in this study are shown in Figure
4.2 A and B. A semivariogram describes the spatial correlation between the different locations at which a random variable (e.g. HK) is known. The semivariogram is calculated by taking the square of half of the difference between two hydraulic conductivity observations, which are separated by a specific distance (Matheron, 1963). The semivariogram has been calculated using both the GMS and Surfer15 software packages. The level of misfit is not unexpected considering the heterogeneous nature of the study area. The spatial variability of SY and mRECH are assumed to follow the same semivariogram as the log of HK. The streambed conductance (HCOND), roughness coefficient (ROUGHCH), and incision (INCISN) vary for each segment.

Since the model is uncalibrated, the parameter values are based on available data and expert knowledge. The HK and SS values used to derive the variograms are based on aquifer test (pump test) data provided by GNS Science. The SY, ROUGHCH, HCOND, and INCISN parameter values are based on expert knowledge.

![Semivariogram (black) and the model variogram (red) for A) log of Hydraulic Conductivity, and B) log of Specific Storage.](image)

**Figure 4.2.** Semivariogram (black) and the model variogram (red) for A) log of Hydraulic Conductivity, and B) log of Specific Storage.

### 4.1.2 Predictions

The analysis of the parameter and predictive uncertainty surrounding water quantity predictions, and the analysis of the value of data in reducing such uncertainties was performed for two locations: the outlet from the Mataura river at Gore, which occurs at the bottom of the entire catchment, and at the outlet from McKellar Stream, which is a spring-fed stream in the middle of the catchment (Figure 4.3). In order to explore the worth of data in the context of stream depletion three additional pumping wells are added (locations shown in Figure 4.3). The pumping rate in all three wells is 200 m$^3$/day for 6 months per year (January-June); the pumping rate is zero for the remainder of the year. The rate and well locations were chosen to get a significant impact on the streamflow in the form of stream depletion. Figure 4.4 show the percentage difference in streamflow between the original model and the scenario with extra pumping.

In order to successfully apply the data worth method when investigating predictions concerning stream depletion there has to be a significant difference in streamflow between the original flow and the streamflow when extra pumping takes place (at least 5% difference). This difference ensures that the derivatives are significantly high enough. Figure 4.4 A shows the impact of seasonal groundwater pumping on the streamflow. During the season where no additional pumping takes place the percentage...
difference returns to 0% meaning that the discharge returns to its original amount. Figure 4.4 B shows the same comparison for McKellar Stream. The percentage difference in streamflow is larger for McKellar Stream than at Gore. In addition, the percentage difference no longer recovers to 0% difference in stream flow, when pumping ceases. This could be attributed to the fact that McKellar Stream is spring-fed, and has a much smaller discharge than the Mataura river at Gore such that the pumping rate creates a proportionally larger stream depletion effect, and so the stream and the aquifer from which it is sourced does not have sufficient time to return to the original discharge rates that occur during the season with no pumping.

As described in the introduction, three predictions concerning stream depletion are investigated:
- The first prediction, is the difference in the number of days below the Q95 flow caused by the additional pumping wells.
- The second prediction relates to the difference in the maximum number of consecutive days below Q95 caused by the additional wells.
- The third prediction is the magnitude of stream depletion (in terms of flow rates) as a result of additional pumping. With the help of Figures 4.4 A and B and the modelled time series of discharge, it was determined that the maximum difference in discharge in the model occurred on 2013-06-28. The third prediction considered is therefore the magnitude of stream depletion on 2013-06-28.
4.1.3 Parameterisation Simplifications
The impact of model parameterisation simplification on the spatial distribution of the worth of additional groundwater telemetry data is investigated for the prediction number of days below Q95 and the magnitude of stream depletion prediction. The simplification of interest considered was spatial parameterisation density. Three spatial parameter density scenarios were investigated: 1) pilot-points, 2) homogeneous, 3) grid-cell based parameterisation.

- Scenario 1) contains the original parameterisation density based on pilot-point parameterisation for HK, SS, and SY (350 parameters each), described in detail above.
- Scenario 2) has the parametrisation for HK, SS, and SY as homogeneous, this means that HK, SS, and SY are represented by one parameter each for the entire model domain.
- Scenario 3) contains a grid-cell based parameterisation for HK, which means that parameters for HK are assigned to each model grid cell (11,077 parameters). The SS and SY are based on pilot-point distribution (350 parameters each).

4.1.4 Data
For the water quantity section of the study, the worth of four different types of existing data are investigated (Table 4.1). The number of observation locations and record length vary widely and is listed for each data type in Table 4.1. The additional data is discussed in section 4.3.3 Additional Data.

Table 4.1, Different data types available, their abbreviations used in this study, the number of observation locations and the record lengths.

<table>
<thead>
<tr>
<th>Data type</th>
<th>Abbreviation</th>
<th>Number of observation locations</th>
<th>Number of observations per site/Record length</th>
</tr>
</thead>
<tbody>
<tr>
<td>Groundwater level</td>
<td>gw_level</td>
<td>185</td>
<td>1 – 176 observations</td>
</tr>
<tr>
<td>Groundwater telemetry</td>
<td>gw_telem</td>
<td>7</td>
<td>0.7 – 11.6 years</td>
</tr>
<tr>
<td>Surface water streamflow</td>
<td>sw_strmflow</td>
<td>4</td>
<td>0.6 – 5.1 years</td>
</tr>
<tr>
<td>Surface water loss and gains</td>
<td>sw_lossgain</td>
<td>11</td>
<td>2 – 8 observations</td>
</tr>
</tbody>
</table>

4.2 Water Quality

4.2.1 Transport Model
The transport model used in this study was developed by GNS Science. Nitrate transport is simulated using the software MT3D – USGS (Bedakar, 2016). The transport model uses the output from the uncalibrated 1-layer steady state version of the groundwater flow model described in section 4.1.1 Groundwater Flow Model. The transport model is a pseudo-steady state model, which means in this case that it runs for 100 years with increasing time step length with constant boundary conditions until the outputs remain constant over time. The transport model used in this study is uncalibrated. The initial model set up was configured using the graphical user interface GMS. After that the MT3D packages were altered using a text editor and the Python package FloPy.

The amount of nitrate loading (mg/L) is specified in the Source-Sink Mixing (SSM) package and consists of the 2010-2015 average of the nitrate loading data provided by Environment Southland.

In addition to the uncertainty associated with the parameters discussed in 4.1.1 Groundwater Flow Model, the uncertainty associated with transport simulation parameters denitrification (DEN), dispersivity (DISP), and porosity (PORO) are also considered in this part of the study. The DEN and PORO are spatially parameterised using the pilot-points and HK variogram described in 4.1.1 Groundwater Flow Model. DISP is characterised using three parameters: one for longitudinal dispersivity (AL), one for horizontal transverse dispersivity (TRPT), and one for the vertical transverse dispersivity (TRPV).

Since the transport model is uncalibrated, the parameter values are again based on available data and expert knowledge. The DISP and PORO values are based on expert knowledge. The DEN rates are
based on a combination of data provided by the New Zealand Institute of Environmental Science and Research Limited (ESR) and expert knowledge.

4.2.2 Prediction and Locations
The analysis of the parameter and predictive uncertainty surrounding the water quality prediction and the value of the data in reducing such uncertainties was performed for seven locations: four surface water locations and three groundwater locations (Figure 4.5). The four surface water locations represent key periphyton monitoring locations (Figure 4.5 A and B). Jacobstown and Cooper’s Bore are town water supply bores, and N Well is an additional hypothetical well location added to explore the difference in worth of data for the difference in groundwater nitrate concentration between upstream and downstream wells.

In order to explore the worth of data in the context of an increase in nitrate as a result of land-use changes, the initial nitrate concentration is doubled, this is achieved by altering the multiplier in the SSM package.

4.2.3 Data
The data worth analysis for the water quality aspect of this study is performed on the same data as already outlined in section 4.1.4 Data (Table 4.1) plus an eleven additional concentration data types (Table 4.2). Since the transport model is pseudo-steady state, the observations listed in Table 4.1 and 4.2 are temporally averaged. The number of water quality observation locations is listed in Table 4.2.

<table>
<thead>
<tr>
<th>Data type</th>
<th>Abbreviation</th>
<th>Number of observation locations</th>
</tr>
</thead>
<tbody>
<tr>
<td>Groundwater tritium</td>
<td>g1_tr</td>
<td>10</td>
</tr>
<tr>
<td>Groundwater nitrate</td>
<td>g2_n</td>
<td>124</td>
</tr>
<tr>
<td>Groundwater chloride</td>
<td>g3_cl</td>
<td>152</td>
</tr>
<tr>
<td>Groundwater delta $^{13}$C</td>
<td>g4_d13c</td>
<td>29</td>
</tr>
</tbody>
</table>

Figure 4.5, Study area with the nitrate locations. A) Complete study area with the outline of the catchment (red line), the groundwater nitrate concentration locations (red dots) and the surface water nitrate concentration (red lines along the river) including the names of the study locations. B) A close up of the upstream surface water concentration locations (red lines along the river) including their names.
4.3 Modelling Strategy
In order to conduct the data worth analysis a number of distinct steps, as described below, are involved.

4.3.1 Model Set-Up
The modelling set-up was supported by both Python code and partly using the Windows Command Prompt for the PEST utilities (Doherty, 2018). A PEST control file, the MODFLOW and MT3D package files and model batch files were provided by GNS Science, which were then altered for this study. Separate PEST control files were used for the water quantity and quality section of this study.

The MODFLOW packages were investigated and altered using the python suite of codes ‘FloPy’ (Bakker et al., 2016). The additional pumping wells were added to the WEL package. The flow model is run three times: once to obtain the initial starting heads, the original model, and the model with additional wells.

For the water quality section, the steady state MODFLOW – NWT model is run followed by the original MT3D model, and then finally the MT3D model with double the nitrate loading.

4.3.2 Predictions
The difference in the number of days below Q95 is calculated using the PEST utilities BUD2SMP, TSPROC, and OBS2OBS. BUD2SMP extracts the streamflow time series from the MODFLOW output file, TSPROC calculates the amount of days below the Q95, and OBS2OBS calculates the difference between the amount of days below Q95 for the different model runs. The maximum number of consecutive days below Q95 is calculated using the PEST utility CONDAYLESS. After that, the difference in consecutive days is calculated using OBS2OBS. The magnitude of the depletion rate, as well as the difference in discharge between the original model and the model with additional wells, is calculated using TSPROC. The difference in nitrate concentrations is calculated using MOD2SMP, to extract the concentration data, and OBS2OBS to calculate the difference. Once all the predictions are calculated, they are added to the PEST control file.

4.3.3 Additional Data
Additional new observations wells are added in every 10th cell, in total 111 new wells, to assess the worth of possible future data acquisition efforts. For the water quantity section of the study the new possible data analysed is comprised of daily groundwater telemetry data over a single year, 2014.

In addition, alternate temporal monitoring scenarios are also investigated for the complete study period (15 years) in every 10th, 20th, or 30th cell and data in every 10th cells on a daily, weekly, monthly, and annual resolution for the complete study period. This allows for the investigation of both a less spatially dense monitoring network and the effects of less frequent monitoring.

In the water quality section of the study the worth of additional nitrate concentration observations in both wells and surface water reaches are explored. The groundwater nitrate concentrations are added in the same locations as the additional telemetry data (every 10th cell). The additional surface water nitrate observations are added in every reach (in total 1204 new observations). Since the transport model is pseudo steady-state the worth of additional new concentration data is only explored in a spatial context.
4.3.4 Establishing Prior Parameter Uncertainty

As described in section 3.2.2 Data Worth Method, in order to calculate worth of additional data the predictive uncertainty, expressed as a variance, of a specific prediction of interest is needed. In order to calculate the data worth, the proportional decrease in uncertainty that is accrued when additional information is considered in comparison to the initial (prior) uncertainty (eq. 4.8). Thus, the first step is to establish the prior parameter uncertainty, which is then propagated through the model to yield the prior predictive uncertainty using eq. 4.8. The prior parameter uncertainty, in the form of the standard deviation, of the ROUGHCH, HCOND, and INCISN are based on expert knowledge. To represent the spatial correlation of HK, SS, SY and mRECH as well as the uncertainty associated with these parameters, covariance matrices are used. These were configured using the PEST utility PPCOV and the variograms described in section 4.1.1 Flow Model. PPCOV produces a covariance matrix based on a pilot-points file and a geostatistical structure file (Watermark Numerical Computing, 2016). The parameter standard deviation used for the definition of the prior parameter uncertainties are summarised in Table 4.3, the covariance structures used can be found in Appendix A.1.

Table 4.3. Parameter standard deviations used for the definition of the prior parameter uncertainties.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Standard Deviations</th>
</tr>
</thead>
<tbody>
<tr>
<td>ROUGHCH</td>
<td>6e-6</td>
</tr>
<tr>
<td>HCOND</td>
<td>0.17 m/d</td>
</tr>
<tr>
<td>INCISN</td>
<td>0.01 m</td>
</tr>
<tr>
<td>AL</td>
<td>0.35 m</td>
</tr>
<tr>
<td>TRPT</td>
<td>0.35 %</td>
</tr>
<tr>
<td>TRPV</td>
<td>0.35 %</td>
</tr>
</tbody>
</table>

4.3.5 Observation Weights

The next step is to assign the observation weights to each observation. The observation weights are used to produce the covariance matrix of the observation error terms (comprising measurement and structural (epistemic) noise) (C(e)). In this process, it is assumed that the inverse of the weight is equivalent to the standard deviation of the noise (Watermark Numerical Computing, 2016). In order to obtain the observation weight, the PEST utility PWTADJ2 is used. This utility reads both the current objective function and the contribution of each observation group to this objective function from a run record file. By using PWTADJ2 observation weights are reassigned on the basis of the measurement and the structural noise, allowing them to be consistent with the theoretical underpinnings of the linear uncertainty analysis method adopted in this study.

4.3.6 Computing the Jacobian Matrix

As described in 3.2 Data Worth Method the Jacobian (or sensitivity) matrix contains information about the relationship between the model outputs and parameters and, in this study, provides the basis for the uncertainty analysis (Watermark Numerical Computing, 2016). A ‘relative’ central difference methodology was adopted for calculating derivatives, meaning that that for every parameter, the step used for the forward-difference calculation of derivatives is computed as a fraction of the current value of the parameter (Watermark Numerical Computing, 2016). Within the PEST software, the size of the derivative fraction was fixed and determined by the parameters ‘DERINC’ and ‘INCTYP’ (Watermark Numerical Computing, 2016).

4.3.7 Uncertainty analyses

Figure 4.6 shows the workflow adopted that combined both the PEST and pyEMU (White et al., 2018) (pyEMU is a python-based framework that builds on and extends PEST) software platforms. Note that this workflow was similar for both the water quantity and water quality section of this study. Using PEST, the first step in the uncertainty analyses process is running a PEST utility GENLNPRED. GENLINPRED is short for ‘generalized linear predictive uncertainty/error analyser’ (Watermark Numerical Computing, 2016). Running this programme prompts a series of questions which lets the user decide which aspects of uncertainty analyses should be considered. GENLINPRED calls a variety of additional PEST utilities that will then carry out the selected analyses and retrieves the input files required for them.
One of these utilities, IDENTPAR is run to calculate the parameter identifiability. The parameter identifiability is prediction independent and provides information about how well the parameters are able to be estimated by the existing dataset (Watermark Numerical Computing, 2016). The parameter identifiability is calculated on a scale of 0, non-identifiable, to 1, completely identifiable. For a more detailed description of the calculation of the parameter identifiability see Doherty (2015).

Another utility, PREDUNC4 is used to calculate the pre- and post-calibration parameter contributions to predictive uncertainty (Watermark Numerical Computing, 2016). This analysis is performed for the number of days below Q95 prediction, the magnitude of stream depletion prediction and the difference in nitrate concentration prediction.

The PREDUNC5 utility is used to calculate the change in uncertainty when observations are added and subtracted (Watermark Numerical Computing, 2016). The change in uncertainty is calculated for the observation groups and the individual observation locations for both the existing data and the additional new data for all predictions. The spatial data worth analysis for the additional new telemetry data is also performed using the homogeneous and grid-cell based parameterisation for the number of days below Q95 and the magnitude of stream depletion predictions.

The same algorithms incorporated in PREDUNC 4 & 5 can be implemented by pyEMU (See Appendix A.2). As shown in Figure 4.6 the equivalent of PREDUNC4 in pyEMU is ‘sc.get_par_contribution()’, and the equivalent of PREDUNC5 addition is ‘sc.get_added_obs_group_importance()’, and PREDUNC5 subtraction is ‘sc.get_removed_obs_group_importance()’. In pyEMU an additional function called “next_most_important_added_obs()” is used in order to calculate the order of the first new observation that would reduce the initial uncertainty the most. This function considers the existing data, which PREDUNC5 does not.

The processing and visualizing of the results are done with a combination of Surfer 15, Excel 2016, and Python. The PREDUNC4 outputs are normalized by transforming it into a percentage of the total pre-calibrated uncertainty. The PREDUNC5 and pyEMU outputs are transformed into a proportional reduction off the prior uncertainty.

Figure 4.6, Flow chart displaying the workflow with both PEST and pyEMU. Arrows in the middle indicate the part of the software that is the equivalent of each other.
4.4 Assumptions
The data worth method is based on two important assumptions: 1) the model shows linear behaviour, and 2) the uncertainty can be characterised using Gaussian distributions (Dausman et al., 2010; Wallis et al., 2014). A model shows linear behaviour if its derivative remains consistent over changing parameter values. Because of the stochastic nature of groundwater models, this assumption does not always hold. Herckenrath et al. (2011), used both the null-space Monte Carlo (NSMC) method and FOSM to quantify uncertainty. They show that both methods encapsulate the truth but that the FOSM method overestimated uncertainty for the example examined. Since the focus of the data worth method is to investigate the relative reduction in uncertainty achieved by different observations, the absolute magnitude of standard deviation of the predictive uncertainty is of less importance, and instead it is the relativity of uncertainty reductions that must be robust.

The models used in this study are a highly-simplified version of the real-world aquifer system. Because of the coarse cell size (250 m by 250 m) the small-scale heterogeneity of the system is lost. Despite this, they are still suited for the predictions that are investigated in this study, as the predictions being investigated consider larger, catchment scale, processes. The single layer model is also appropriate because of the thin nature of the aquifer.
5. Results

The first part of this results section focusses on the water quantity section which analyses parameter identifiability and data worth analyses. This is followed by a section which presents the results for the water quality data worth analyses. The results below were all based on the model with the pilot-point based parameterisation of HK, SS, SY, and mRECH unless otherwise stated.

5.1 Water Quantity

The water quantity results principally relate to the exploration of data worth in terms of informing the low flow predictions described in section 4.1.2 Predictions.

5.1.1 Parameter Identifiability

Figure 5.1 A to D show the spatial distribution of parameter identifiability values for the mid-Mataura catchment, based on the available monitoring data used in the water quantity model calibration (e.g. stream flows, groundwater levels and stream-aquifer loss and gain data) for the following parameter distributions: A) HK, B) SY, C) mRECH, and D) SS. Recall that if a parameter has an identifiability of 0, then there is no information in the calibration dataset to inform that parameter value. In contrast, if a parameter has an identifiability of 1, then it is uniquely estimable on the basis of the calibration dataset. Its estimation will still be accompanied by uncertainty related to measurement and model structural noise, but not from a deficit of information in the calibration dataset. If a parameter has an identifiability that is between 0 and 1, this indicates that information pertinent to that parameter resident in the calibration dataset is shared between this parameter and at least one other parameter.

The black dots in the figures are existing groundwater level observations and the purple dots existing groundwater telemetry data. Identifiability values range from 0, not identifiable (blue) to 1, identifiable (red). Overall, in all figures the blue colours prevail, this indicates that the parameters were generally not well informed. More yellow and orange colours are present in Figure A compared to the other figures, indicating that, with the existing monitoring data, spatially distributed HK parameters were significantly better informed compared to the other parameters examined. The HK parameters which were better informed (more yellow and orange colours) were located in areas of more dense monitoring wells networks. The parameters which appear to be least informed by the existing monitoring data were the mRECH parameters (identifiability ranges from 5.54E-06 to 1.64E-02). Note that parameter identifiability alters if additional data is included in the monitoring network and model calibration. While this change in identifiability with more data was not explored in this thesis, it is this change that underpins the results in the data worth analysis, which is not described.
Figure 5.1. Parameter identifiability A) HK, B) SY, C) mRECH, D) SS. Red outline shows the catchment area, blue lines represent streams present in the study area. Black dots indicate existing groundwater level observation locations, purple dots show telemetry data locations. The colours filling the catchment are on a scale between 1, identifiable (red) to 0, not identifiable (blue).
5.1.2 Parameter Contribution to Uncertainty

Figure 5.2 A to D show the pre- and post-calibration parameter-group contribution to uncertainty for difference in number of days below the Q95 flow prediction and the magnitude of stream depletion prediction. The scale on the y-axis are prediction specific, as such the graphs should not be compared to each other directly, however, relative patterns can be compared. From the different graphs in Figure 5.2 the HK parameter group was shown to have the largest contribution to uncertainty for both the days below Q95 and magnitude of stream depletion prediction, as well as the largest reduction in uncertainty through calibration to observation data. Looking at the y-axis of the graphs the contribution by HK was especially large for McKellar Stream (5.2 B and D) and relatively much smaller at Gore (5.2 A and C). It was also clear the SS and SY contribute relatively more to uncertainty when predicting the days below Q95 at Gore, compared to when predicting the days below Q95 at McKellar Stream and when prediction the magnitude of stream depletion at both Gore and McKellar Stream. mRECH, HCOND and INCISN all have a small contribution to uncertainty for both the days below Q95 and magnitude of stream depletion prediction at both locations. What stands out was that the post-calibration contribution to uncertainty for mRECH in A, B and C and HCOND in B was larger than the pre-calibration contribution to uncertainty, this will be discussed further in section 6.2.1.2 Increase in Post-Calibration Uncertainty Contribution.

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5.1.3 Data Worth of Existing Data

5.1.3.1 Observation Groups

Figure 5.3 A to F show the change in uncertainty when the different observation groups from all the existing monitoring data, were either (i) added (blue) to a base of no monitoring data or (ii) subtracted (green) from the complete monitoring dataset. It was clear that the change in uncertainty when adding
the observations was always larger than when subtracting. The patterns for Figures 5.3 A, D, and E were very similar, as well as the patterns for Figures 5.3 B and F. For the Figures A, D, and E the gw_telem data causes the largest reduction in uncertainty (maximum reduction in uncertainty between 37% and 83%), recall that this data has the most frequent temporal measurements in the monitoring dataset. For the Figures B (days below Q95 at McKellar Stream) and F (magnitude of stream depletion at McKellar Stream) the sw_strmflow data provides the largest reduction in uncertainty (maximum reduction of 68% for B and 39% for F). The Figure 5.3 C shows a unique pattern, indicating that the gw_level data, which has the greatest spatial distribution of available measurements, causes the largest reduction in uncertainty (maximum reduction in uncertainty of 67%).

Figure 5.3. Reduction in uncertainty when the observation groups were subtracted (green) and added (blue) for A) Difference in days below Q95 at Gore, B) Difference in days below Q95 at McKellar Stream, C) Difference in number of consecutive days below Q95 at Gore, D) Difference in number of consecutive days below Q95 at McKellar Stream, E) Magnitude of stream depletion at Gore, and F) Magnitude of steam depletion at McKellar Stream.
5.1.3.2 Spatial Data Worth Existing Groundwater Level Data
Figures 5.4 A to F depict how the worth of existing groundwater level data was spatially distributed when considering the addition of data, recall that this calculation assumes that the addition of each monitoring well data set was considered in isolation, rather than in combination with other data. The spatial distribution of the data worth, given the subtraction of the groundwater level data from an otherwise complete monitoring dataset is shown in Appendix A.3. The colours represent the decrease in uncertainty on a scale of 0 (blue) to 1 (red) the colour scale is the same throughout all the following spatial data worth plots (both the water quantity and water quality) to allow direct comparison between areas of high and low data worth in the figures. The dots sizes are proportional to the decrease in uncertainty and are prediction specific and therefore should not be compared between figures. What stands out the most for these figures was that Figures A, C and E (low flow predictions at Gore) have very similar patterns, as well as Figures B and F (days below Q95 and magnitude of stream depletion at McKellar Stream). For the Figures A, C, and E, the groundwater level observations in the upstream portion of the catchment were shown to significantly reduce the predictive uncertainty. With a maximum reduction in uncertainty of 20% for A, 35% for B, and 30% for C. For Figures B, D and F, the single groundwater level observation closest to McKellar Stream reduces the uncertainty the most (19% for B, and 25% for F), with groundwater level observations in the upstream region also contributing to predictive uncertainty reduction. The groundwater level observations reduce the uncertainty the least for the difference in consecutive days below Q95 prediction for McKellar Stream, the maximum reduction in uncertainty was 6% (Figure 5.4 D).

5.1.3.3 Spatial Data Worth Existing Groundwater Telemetry Data
Figures 5.5 A to F show the spatial data worth for addition of existing telemetry data for the low flow predictions once again using the addition version of the data worth analysis. The spatial distribution of the data worth analysis using the subtraction method for the groundwater telemetry data is shown in Appendix A.4. The numbers in Figure 5.5 A represent the length of the record in years. Figure 5.5 A, C, and E (low flow predictions at Gore) have very similar pattern. Again, the upstream area reduces the predictive uncertainty significantly for the predictions at Gore (maximum reduction in predictive uncertainty of 38% for C and 59% for E). The groundwater telemetry observation location downstream, where the different sub-streams converge, appears to reduce the uncertainty the most for Figure 5.5 A (73% reduction in uncertainty). After that, the telemetry data locations upstream, particularly to the northeast reduce the uncertainty the most. The patterns for Figure 5.5 B, D and F (low flow predictions at McKellar Stream) were similar as well. The telemetry location upstream from McKellar Stream reduces the uncertainty the most in these figures (maximum reduction of 60% for B, 34% for D, and 48% for F).
Figure 5.4. Proportional reduction in uncertainty after the addition of existing groundwater level data for all the predictions: A) Difference in days below Q95 at Gore, B) Difference in days below Q95 at McKellar Stream, C) Difference in number of consecutive days below Q95 at Gore, D) Difference in number of consecutive days below Q95 at McKellar Stream, E) Magnitude of stream depletion at Gore, and F) Magnitude of stream depletion at McKellar Stream. The colours are on a scale of 0 (blue) to 1 (red) and are the same for all figures. The dots show the groundwater level observation locations and the sizes of the dots are proportional to the percentage decrease in uncertainty and are prediction specific. The black dots with white circles around them are the additional wells and the red dots are the prediction locations.
Figure 5.5, Proportional reduction in uncertainty after the addition of the existing groundwater telemetry data for all the predictions: A) Difference in days below Q95 at Gore, B) Difference in days below Q95 at McKellar Stream, C) Difference in number of consecutive days below Q95 at Gore, D) Difference in number of consecutive days below Q95 at McKellar Stream, E) Magnitude of stream depletion at Gore, and F) Magnitude of steam depletion at McKellar Stream. The colours are on a scale of 0 (blue) to 1 (red) and are the same for all figures. The dots shown are the groundwater telemetry observation data locations. The sizes of the dots are proportional to the percentage decrease in uncertainty and are prediction specific. The numbers in A) represent the length of the observation period in years. The black dots with white circles around them are the additional wells and the red dots are the prediction locations.
5.1.3.4 Data Worth of Existing Streamflow Data

The change in uncertainty when adding (blue) or subtracting (green) the individual streamflow-location data for the difference in days below Q95 and the magnitude of stream depletion predictions at Gore and McKellar is shown in Figure 5.6 A to D.

What stands out the most was that for both the days below Q95 and magnitude of stream depletion prediction at both locations was that the addition of the Mataura streamflow data had by far the largest impact (63% to 69% reduction in uncertainty). For both the days below Q95 and magnitude of stream depletion prediction, Waimea and Meadow Burn Stream also afford a reduction between 3% and 8%, while Waikaia observation reduce the uncertainty with less than 0.7%.

Figure 5.6, Proportional change in uncertainty after streamflow observations at Mataura, Meadow, Waikaia, and Waimea were subtracted (green) and added (blue). A) Difference in days below Q95 at Gore, B) Difference in days below Q95 at McKellar Stream, C) Magnitude of stream depletion at Gore, D) Magnitude of stream depletion at McKellar Stream.
5.1.4 Data Worth of Additional Data

5.1.4.1 Worth Observation Groups with Additional Data

Figure 5.7 shows the proportional change in uncertainty after each observation group was added (blue) and subtracted (green); these groups consist of the existing and the additional data (“add_well”). The figures are the same as the graphs in Figure 5.3, plus the new observation group containing the additional telemetry observations in the “add_well” group. The new wells were added in every 10th cell with daily telemetry data for 2014. From Figure 5.7 A to F, it was clear that the potential group of additional wells (in “add_well”) would change the uncertainty the most significantly for the low flow predictions; both when add_well was subtracted and added and will result in a reduction in uncertainty between 63% and 91%.

Figure 5.7, Change in uncertainty when the observation groups were subtracted (green) and added (blue) for A) Difference in days below Q95 at Gore, B) Difference in days below Q95 at McKellar Stream, C) Difference in number of consecutive days below Q95 at Gore, D) Difference in number of consecutive days below Q95 at McKellar Stream, E) Magnitude of stream depletion at Gore, and F) Magnitude of stream depletion at McKellar Stream.
5.1.4.2 Spatial Data Worth with Additional Data

Figures 5.8 A to F show the spatial change in uncertainty after the new additional telemetry wells (e.g. the “add_well” group) were added. The spatial change in uncertainty after the subtraction of the new data can be found in Appendix A.5. The numbers in the plots in Figure 5.8 show the order of the next ten new additional data points that will reduce the uncertainty the most, considering the already existing observation dataset.

Figure 5.8 A, C and E (low flow predictions at Gore) show very similar patterns in terms of colour shading. In these figures the observation point downstream, where the separate streams converge, reduces the uncertainty significantly (between 25% and 75%). Apart from that, the observations upstream, particularly in the northeast, reduce the uncertainty the most (between 30% and 40%). The observations located in the northwest section reduce the uncertainty much less compared to the other observations upstream. The order of the most important “next observation” for Figures A and C are identical and are spread out through the middle and north part of the catchment. Figure 5.8 E shows a unique pattern in terms of the distribution of the next most important added observations, the pattern was in the same area as the yellow colour shading.

Figures 5.8 B, D, and F (low flow predictions at McKellar Stream) also show very similar patterns in terms of colour shading. The observations that reduce the uncertainty the most were centred around McKellar Stream in all three figures (maximum reduction in uncertainty between 38% and 59%). The order of most important added observation was identical for Figure B and D. The next most important added observations were all centred around the upstream section of McKellar Stream, and partly surrounding the Waimea river. The next most important added observation pattern in Figure 5.8 F was unique. In this figure, the next most important observations were not in the same area as the yellow colour shading, but instead spread out over the middle and western section of the catchment.
Figure 5.8. Proportional reduction in uncertainty after addition of the new additional groundwater telemetry wells. The colours are on a scale from 0 (blue) to 1 (red) and the same scale is used for all figures. The black dots show the location of the new additional well and the sized of the dots are proportional to the reduction in uncertainty and are prediction specific. The numbers show the order of the next new observation that will reduce the uncertainty the most. The black dots with white circles around them are the additional wells and the red dots are the prediction locations. A) Difference in days below Q95 at Gore, B) Difference in days below Q95 at McKellar Stream, C) Difference in number of consecutive days below Q95 at Gore, D) Difference in number of consecutive days below Q95 at McKellar Stream, E) Magnitude of stream depletion at Gore, and F) Magnitude of steam depletion at McKellar Stream.
5.1.5 Diminishing Return Plots for Additional Data

The diminishing returns of additional monitoring wells at increasing spatial frequencies and/or increasing temporal monitoring frequencies was examined in this section. The diminishing return plots are shown in Figure 5.9 and 5.10 for the difference in days below Q95 and the magnitude of stream depletion predictions at Gore and McKellar Stream. These plots were plotted on the same scale respectively and thus can be compared directly.

5.1.5.1 Spatial Diminishing Return Plots

Figure 5.9 shows the reduction in uncertainty when daily telemetry data for the complete study period (15 years) was added in every 10th, 20th, and 30th model cell. Figures A and B show that the reduction in uncertainty remains similarly high when reducing the spatial distribution of the additional data (from left-to-right in Figure 5.9). The reduction in uncertainty for 5.9 A goes from 99.98% to 99.94% (left to right), and for 5.9 B from 99.99% to 99.96% (left to right).

In contrast, the effect of reducing the numbers of observation wells in term of a decrease in predictive uncertainty reduction can be seen in Figures C and D (the magnitude of stream depletion at Gore and McKellar). They show that when wells were present in every 20th or 30th cell the reduction in uncertainty diminishes, but still remains high. In Figure 5.9 C the uncertainty reduction goes from 97.26% to 87.89% (left to right), and in Figure 5.9 D it goes from 93.13% to 68.22% (left to right).

![Figure 5.9. Spatial diminishing return plots. Proportional reduction in uncertainty after adding daily telemetry data for the complete model time (15 years) in every 10th, 20th, and 30th cells. A) Difference in days below Q95 at Gore, B) Difference in days below Q95 at McKellar Stream, C) Magnitude of stream depletion at Gore, D) Magnitude of stream depletion at McKellar Stream.](image-url)
### 5.1.5.2 Temporal Diminishing Return Plots

The temporal diminishing return plots are shown in Figure 5.10 A to D. It shows the reduction in uncertainty for the additional wells located in every 10th cell with daily, weekly, monthly or annual record frequencies for the complete study period (15 years).

Figure 5.10 A and B (difference in days below Q95 at Gore and McKellar Stream) show the least change in reduction of uncertainty after decreasing the measurement frequency; the reduction in uncertainty remains very high for the annual frequency. The reduction in uncertainty for 5.10 A goes from 99.98% to 99.86% (left to right), and for 5.10 B from 99.99% to 99.96% (left to right).

In contrast, the reduction in uncertainty was clearly impacted by varying measurement frequencies in Figures 5.10 C and D (the magnitude of stream depletion at Gore and McKellar). There appears to be a consistent decrease in uncertainty-reduction when going from daily to weekly, to monthly (97.26% to 93.45% for 5.10 C and 93.13% to 85.71% for 5.10 D), followed by a sudden drop to a percentage reduction of 83.36% for 5.10 C and 73.36% for 5.10 D when the measurements were taken once a year.

![Temporal Diminishing Return Plots](image)

**Figure 5.10.** Temporal diminishing return plots. Proportional reduction in uncertainty after adding groundwater telemetry data in every 10th cell with daily, weekly, monthly or annual data for the complete study period. A) Difference in days below Q95 at Gore, B) Difference in days below Q95 at McKellar Stream, C) Magnitude of stream depletion at Gore, D) Magnitude of stream depletion at McKellar Stream.

### 5.1.6 Simplification

The extent to which different parameterisations (grid-cell, pilot-point based or homogeneous) impacts the outcomes, and therefore the validity, of the data worth analysis was explored in this section. Note that the grid-cell based parameterisation would be considered to allow the greatest representation of the ‘real world’ heterogeneity within this model setup.
Figures 5.11 A to D and 5.12 A to D show the results of the spatial data worth of the 1 year of additional daily telemetry data in every 10th cell based on homogeneous parameterisation and grid-cell based parameterisation, respectively.

### 5.1.6.1 Spatial Data Worth Using a Homogeneous Parameterisation

By comparing Figure 5.11 (homogeneous parameterisation) to Figure 5.8 (pilot-point parameterisation) it was clear that the use of a homogeneous parameterisation scheme produces a drastically different data worth pattern. This was especially the case for Figures 5.11 B, C, and D: almost all the observations seem to significantly reduce the uncertainty (70% - 99%) apart from the area around the upstream section around the Mataura river. Figure 5.11 A, while also showing a more uniformly high distribution of data worth, indicates that the additional new observation wells in the northwest corner of the study area will reduce uncertainty the most.

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Figure 5.11. Proportional reduction in uncertainty after addition of new telemetry wells in every 10th cells for daily data during 2014. Based on the model with homogeneous parameterization of HK, SS, and SY throughout the catchment. Colour indicates proportional reduction on a scale of 0 (blue) to 1 (red). The black dots show the location of the new additional well and the sized of the dots are proportional to the reduction in uncertainty and are prediction specific. The black dots with white circles around them are the additional wells and the red dots are the prediction locations. A) Difference in days below Q95 at Gore, B) Difference in days below Q95 at McKellar Stream, C) Magnitude of stream depletion at Gore, D) Magnitude of stream depletion at McKellar Stream.
5.1.6.2 Spatial Data Worth Using a Grid-Cell based Parameterisation

Figures 5.12 A to D (grid-cell based parameterisation) show a data worth pattern that was similar to the Figures in 5.8, which were based on the pilot-point parameterisation. For example, for the Figures 5.12 A and C (days below Q95 and magnitude of stream depletion at Gore) the observations in the upstream portion of the catchment, in particular in the northeast appear to reduce the uncertainty the most, together with the observation location where the different streams converge. This pattern was consistent with that in Figure 5.8 A and C.

Figures 5.12 B and D (days below Q95 and magnitude of stream depletion at McKellar Stream) show consistency with Figure 5.8 B and D in that the observation closest to McKellar Stream will reduce the uncertainty the most, and the order of next most important added observations was also centred around McKellar Stream. A difference apparent between the data worth distribution in Figures 5.8 and 5.12 was that the worth of the data was lower when using the grid-cell based parameterisation (more blue/light yellow colour shading) compared to when using the pilot-point based parameterisation (bright yellow shading).

Figure 5.12, Proportional reduction in uncertainty after addition of new telemetry wells in every 10th cells with daily data during 2014. Based on the model with the grid-cell based HK parameterisation and pilot-point based SS and SY parameterisation. Colour indicates proportional reduction on a scale of 0 (blue) to 1 (red). The black dots show the location of the new additional well and the sized of the dots are proportional to the reduction in uncertainty and are prediction specific. A) Difference in days below Q95 at Gore, B) Difference in days below Q95 at McKellar Stream, C) Magnitude of stream depletion at Gore, D) Magnitude of stream depletion at McKellar Stream.
5.2 Water Quality
The water quality results principally relate to the exploration of data worth in terms of informing the nitrate stream and groundwater concentration predictions resulting from land-use change, as described in section 4.3.2 Predictions. Also, recall that additional parameters were added to this water quality focussed analysis, namely denitrification rates (DEN), porosity (PORO) and dispersion (DISP).

5.2.1 Parameter contribution to uncertainty
The pre- and post-calibration parameter contribution to uncertainty for the difference in nitrate concentration prediction for all locations is shown in Figure 5.13 A to G (e.g. nitrate concentrations at surface water sites and in groundwater wells).

Three overall patterns were clear. Firstly, it was evident that the stream parameters HCOND and INCISN have no significant pre-and post-calibration contribution to uncertainty for all prediction locations. Secondly, it also appears that the parameters governing groundwater transport velocities and nitrate attenuation rates e.g. DEN, HK, and PORO play an important role for most, but not all, of the selected water quality predictions (5.13 A, C, D, E, F). Thirdly, the source term, which was incorporated in the data worth analysis via the mRECH parameter group as a recharge concentration, was most important for many but not all predictions. What also stands out was that for some predictions (5.13 A, B, C, D) the post-calibration contribution to uncertainty was larger than the pre-calibration contribution to uncertainty, this will be discussed further in section 6.2.1.2 Increase in Post-Calibration Uncertainty Contribution.

5.2.1.1 Surface Water Predictions
Notwithstanding the general patterns mentioned above, for the prediction of nitrate concentration in the Mataura River at Gore (A) the most important parameter group appears to be the mRECH, followed by the PORO, HK, and DEN parameter groups. The results also indicate that for the prediction of nitrate concentration in the Meadow Burn spring-fed stream at Mataura (B) it was only the mRECH parameter group that contributes significantly to uncertainty.

The DEN, HK, and PORO parameter groups all play a significant role for the surface water concentration prediction at Waimea at Mataura (C), with an emphasis on the PORO parameter group. For the McKellar Stream at Waimea prediction (D), the DEN, HK, mRECH, and PORO parameter groups all play a significant role, with the PORO parameter group contributing the most to the uncertainty.

5.2.1.2 Groundwater Predictions
Cooper’s Bore (E) shows the largest difference between the pre- and post-calibration contribution to uncertainty, indicating that the calibration dataset had the potential to reduce the uncertainty of this prediction more than other predictions, as discussed further in 6.2.2.1 Worth Observation Groups. The parameters that show a significant contribution to uncertainty comes from the DEN, HK, and PORO parameter groups. The well at Jacobstown (F) shows a very similar pattern as Cooper’s Bore (E). The DEN, HK, and PORO all greatly contribute to uncertainty, next to that there was a significant difference between the pre- and post-calibration contribution to uncertainty. The N Well (G) shows the only contribution to uncertainty occur from the mRECH parameter group, and then the DISP, DEN, and PORO groups to a lesser extent.
Figure 5.13. Pre- (blue) and post- (orange) calibration parameter contribution to uncertainty for the prediction: A) Difference in nitrate concentration Mataura at Gore, B) Difference in nitrate concentration Meadow Burn at Mataura, C) Difference in nitrate concentration Waimea at Mataura, D) Difference in nitrate concentration McKellar at Waimea, E) Difference in nitrate concentration at Cooper’s Bore, F) Difference in nitrate concentration at Jacobstown, G) Difference in nitrate concentration at N Well.
5.2.2 Worth Existing Data

5.2.2.1 Observation Groups
The change in predictive uncertainty when the existing observation groups were added (blue) and subtracted (green) are shown in Figure 5.14 A to G. It was clear that the g2_n observation group (groundwater nitrate observations) provide the greatest change in uncertainty (for both addition and subtraction data worth analysis) for all locations. The extent to which it reduces uncertainty differs between the different locations; for Mataura at Gore (A) the reduction was 37%, for Meadow Burn at Mataura (B) and N Well (G) the reduction was between 15% and 19%, and for Waimea at Mataura (C), McKellar at Waimea (D), Cooper’s Bore (E), and Jacobstown (F) the reduction was between 72% and 99%. The next most valuable observation type for all locations was gw_level, apart from 5.14 B (Meadow Burn at Mataura) for which the s2_n observations (surface water nitrate concentration observations) was the most valuable (2.75% reduction). The extent to which the gw_level reduces the uncertainty again varies greatly; for Mataura at Gore (A) the reduction was 26%, for N Well (G) the reduction was between 2.5%, and for Waimea at Mataura (C), McKellar at Waimea (D), Cooper’s Bore (E), and Jacobstown (F) the reduction was between 65% and 93%. After that the sw_lossgain observation group (surface water loss and gain observations) contributes most to uncertainty, followed by the gw_telem and s2_n.
Figure 5.14, Change in uncertainty when the observation groups are subtracted (green) and added (blue) for: A) Difference in nitrate concentration Mataura at Gore, B) Difference in nitrate concentration Meadow Burn at Mataura, C) Difference in nitrate concentration Waimea at Mataura, D) Difference in nitrate concentration McKellar at Waimea, E) Difference in nitrate concentration at Cooper’s Bore, F) Difference in nitrate concentration at Jacobstown, G) Difference in nitrate concentration at N Well.
5.2.2.2 Spatial Worth of Existing Groundwater Concentration Data
The spatial patterns of the reduction in uncertainty achieved as a result of adding in the existing groundwater nitrate concentration data was shown in Figure 5.15 A to G.

Figures 5.15 C, D, E, and F show very similar values and patterns of data worth, with the groundwater nitrate concentration observations that were located downstream, centred around the streams provide the largest reduction in uncertainty (54% to 78% reduction). What also stands out was that a single observation in the south-western part of the study area provides a large reduction in uncertainty (between 24% and 34%) for these prediction locations. This is further discussed in 6.2.2.2 Spatial Worth.

For Figure 5.15 A, Mataura at Gore, the observations downstream, close to Gore and centred around the point where all the streams converge result in the largest reduction in uncertainty (up to 19%).

Figures 5.15 B, Meadow Burn at Mataura, and 5.15 G, N Well, show very similar patterns as well. Looking purely at the colours the reduction in uncertainty was minimal compared to the other figures (maximum reduction between 1.5% and 2.5%), notwithstanding this relatively small reduction in uncertainty the size of the dots indicates that the greatest reduction in uncertainty was achieved by monitoring locations upstream of McKellar Stream and downstream at Gore.

5.2.2.3 Spatial Worth of Existing Surface Water Concentration Data
The reduction in uncertainty as a result of the adding of the existing surface water nitrate concentrations is shown for all locations for the difference in nitrate concentration prediction in Figure 5.16 A, 5.16 B shows the surface water nitrate observation locations. There were more surface water nitrate concentration observations (39 observations) but only the ones that impacted the uncertainty were shown. What stands out was that the observations closer to the outlet of the catchment (mata@Gore, mata@otmi), have a much smaller impact on the uncertainty than observations further upstream (waim@murp, waim@pahi, santrib, waik@waip, waik@waik). The reduction in uncertainty when adding the surface water concentration data was low for all locations and predictions. The reduction in uncertainty was the largest for Mataura at Gore (yellow), 7% reduction. For the other prediction locations, the maximum reduction in uncertainty was between 0.9% and 2.9%.
Figure 5.15. Proportional reduction in uncertainty after addition of the existing groundwater nitrate concentrations for: A) Difference in nitrate concentration Mataura at Gore, B) Difference in nitrate concentration Meadow Burn at Mataura, C) Difference in nitrate concentration Waimea at Mataura, D) Difference in nitrate concentration McKellar at Waimea, E) Difference in nitrate concentration at Cooper’s Bore, F) Difference in nitrate concentration at Jacobstown, G) Difference in nitrate concentration at N Well. Colour indicates proportional reduction on a scale of 0 (blue) to 1 (red). The black dots show the location of the existing groundwater nitrate concentrations and the size of the dots are proportional to the reduction in uncertainty and are prediction specific. The red dots and red in stream lines are the prediction locations.
Figure 5.16, A) Proportional reduction in uncertainty after addition of the existing surface water nitrogen concentration data. The difference in nitrate prediction for Cooper’s Bore (blue), N Well (grey), McKellar at Waimea (light blue), Waimea at Mataura (navy blue), Jacobstown (orange), Mataura at Gore (yellow), Meadow Burn at Mataura (green). B) Streamflow observation locations.
5.2.3 Worth Additional Data

5.2.3.1 Observation Groups

Figure 5.17 A to G depict the change in uncertainty that was achieved by various observation groups, as in Figure 5.14 A to G, but with two new concentration observation groups in surface water and groundwater: add_sw and add_well. The add_sw observation group had the largest impact on the uncertainty for the predictions depicted in 5.17 A, B, D, and G (reduction in uncertainty between 56% and 94%). The second most uncertainty reducing observation group was the existing groundwater data for 5.17 A, B, and D (reducing uncertainty between 13% and 66%). The second most uncertainty reducing group for 5.17 G was the add_well (25% reduction).

It stands out that the reduction in uncertainty for the new additional data groups were not the largest for Figures 5.17 C, E, and F, instead the existing groundwater nitrate concentration group (g2_n) provides the largest impact on the uncertainty (reducing the uncertainty with 76% to 99%).
Figure 5.17. Change in uncertainty when the observation groups are subtracted (green) and added (blue) for: A) Difference in nitrate concentration Mataura at Gore, B) Difference in nitrate concentration Meadow Burn at Mataura, C) Difference in nitrate concentration Waimea at Mataura, D) Difference in nitrate concentration McKellar at Waimea, E) Difference in nitrate concentration at Cooper’s Bore, F) Difference in nitrate concentration at Jacobstown, G) Difference in nitrate concentration at N Well.
5.2.3.2 Spatial Worth of Additional Groundwater Concentration Data

Figure 5.18 A to G show the spatial data worth after the addition of the new groundwater nitrate concentration data. The numbers in the plot show the order of the next most uncertainty reducing observation based on the existing dataset.

The patterns in these figures were very similar to the patterns shown in Figure 5.15, spatial worth of existing groundwater concentration data, in terms of colour shading. The downstream groundwater concentration observations were the most important for the predictions in Figure 5.18 A, C, D, E, F (reduction in uncertainty between 19% and 85%). The maximum reduction in uncertainty for 5.18 B and G was very low, between 1.7% and 2.3%.

The order of next most important observations was scattered around the southern part of the catchment for Figure 5.18 D (McKellar at Waimea) and E (Cooper’s Bore). For 5.18 A (Mataura at Gore) and F (Jacobstown) the order of next most important observations was scattered around the south-western, but upstream, part of the study area. For the prediction depicted in 5.18 C (Waimea at Mataura) the next most uncertainty reducing observations are significantly upstream of the prediction location, in the north-western and north-eastern part of the study area. The order of next most important observations was centred around the prediction location, the middle section of the catchment for Figure 5.18 B (Meadow Burn at Mataura) and 5.18 G (N Well).

5.2.3.3 Spatial Worth of Additional Surface Water Concentration Data

The spatial reduction in uncertainty that can be accrued by new surface water nitrate concentrations is shown in Figure 5.19 A to G. Once again, the numbers indicate the order of the next most important added observation, this time for the first 5 new observations. In these figures the colour scales are prediction dependent and should not be compared directly, however the relative patterns can be compared.

Figures A, C, D, E, F show similar patterns for most of the surface water concentration predictions (except Meadow Burn at Mataura (B)) and for Cooper and Jacobstown bore predictions, which all were located in the lower and western area of the catchment. The surface water concentration data downstream at the point where the different streams converge appears to be the most valuable for all of these predictions (maximum reduction in predictive uncertainty between 14% and 75%). Next to that, it stands out that the concentration data in the Waimea river (southwestern part of the catchment appears to reduce the uncertainty significantly in each of these figures (maximum reduction in uncertainty of 8%).

However, the patterns of the next most uncertainty reducing observations differ for these figures. Figure 5.18 A shows that the observations in the Waimea river were the most important. The same pattern can be seen in Figure 5.18 C. For Figure 5.18 D (McKellar at Waimea), the first five most uncertainty reducing observations were all centred around the prediction location. For 5.18 E (Cooper’s Bore) the next most important added observations were all centred around the point where the different streams converge downstream. For Figure 5.18 F (Jacobstown), the observations alter between downstream where the streams converge and all the way upstream of the Waimea river.

Figure 5.18 B (Meadow Burn at Mataura) and 5.18 G (N Well) share similar patterns in data worth that contrast with those discussed in the above paragraph. The reduction in uncertainty was much smaller (maximum reduction in uncertainty of 9%) than for the predictions discussed in the lower and western part of the catchment. The surface water concentrations that would reduce the uncertainty the most for both predictions were in the middle of McKellar Stream, and the order of the next most important added observations were also centred in this area.
Figure 5.18. Proportional reduction in uncertainty after addition of the additional groundwater nitrate concentration data for: A) Difference in nitrate concentration Mataura at Gore, B) Difference in nitrate concentration Meadow Burn at Mataura, C) Difference in nitrate concentration Waimea at Mataura, D) Difference in nitrate concentration McKellar at Waimea, E) Difference in nitrate concentration at Cooper’s Bore, F) Difference in nitrate concentration at Jacobstown, G) Difference in nitrate concentration at N Well. Colour indicates proportional reduction on a scale of 0 (blue) to 1 (red). The black dots show the location of the new additional well and the sized of the dots are proportional to the reduction in uncertainty and are prediction specific. The number indicates the order of next most important new observation. Red dots and red in stream lines are the prediction locations.
Figure 5.19. Proportional reduction in uncertainty after addition of the additional surface water nitrate concentrations for: A) Difference in nitrate concentration Mataura at Gore, B) Difference in nitrate concentration Meadow Burn at Mataura, C) Difference in nitrate concentration Waimea at Mataura, D) Difference in nitrate concentration McKellar at Waimea, E) Difference in nitrate concentration at Cooper’s Bore, F) Difference in nitrate concentration at Jacobstown, G) Difference in nitrate concentration at N Well. Colour scale indicates proportional reduction and is prediction specific. The number indicates the order of next most important new observation. Red dots and red in stream lines are the prediction locations.
6. Discussion

This chapter will discuss the water quantity results first, followed by a discussion of the water quality results.

6.1 Water Quantity

6.1.1 The Role of Parameters in Uncertainty

Below, first the identifiability of the hydraulic conductivity, storage and recharge parameters are discussed (HK, SS, and mRECH parameter groups). Followed by a discussion of the contribution to the uncertainty of the low flow predictions that was caused by the uncertainty of each parameter group.

6.1.1.1 Parameter Identifiability

Recall that parameter identifiability ranges from 0 to 1, with values of 1 indicating that parameter values can be estimated uniquely. Values of 0 indicate that parameter values cannot be estimated on the basis of the calibration dataset, and their values can only be informed by expert knowledge, and therefore their uncertainty is not reduced by information within the model calibration data-set. Overall, the model parameters (HK, SS, SY, mRECH) were generally not well informed by the existing observation dataset of groundwater levels, stream flows and stream loss and gain data, as evidenced by low parameter identifiability values (Figure 5.1). This result was expected and is consistent with other studies involving groundwater inverse problems (e.g. Knowling et al., 2016; Anar et al., 2017).

The HK parameter group was the most informed by information contained in the model calibration dataset (as indicated by the highest parameter identifiability values). This was because the HK parameter group was informed by the largest observation group in the model calibration dataset, e.g. both long-term groundwater level records as well as single groundwater level observations. In contrast, the SS and SY parameters, which were informed by transient groundwater level information, were less well informed by the model calibration dataset, compared to the HK parameters in this study. This was because there are fewer wells with transient data in this model dataset e.g. more than one groundwater level observation is required to provide information about the storage (e.g., Domenico et al., 1998).

The spatial patterns of higher parameter identifiability coincide with the spatial distribution of the existing observation data. This was specifically seen for the parameter identifiability of the HK (Figure 5.1 A). The parameter identifiability of the SS and SY, generally coincide with areas where longer observation records were present, and storage parameters are able to be informed by transient groundwater level data.

The mRECH parameters were currently the least identified (Figure 5.1 C), there was very little information in the existing dataset that directly informs the mRECH, therefore, the recharge was not uniquely identifiably on the basis of the existing dataset.

6.1.1.2 Parameter Contribution to the Uncertainty of the Low Flow Predictions

The analyses of parameter contribution to predictive uncertainty indicates that the HK parameter group contributed the most to the uncertainty of the low flow predictions examined at both Gore and McKellar Stream. The HK parameter group provides information about how fast water travels through the aquifer and in which direction it flows (for a given hydraulic-head gradient), and since the river baseflow rates are directly related to the aquifer drainage rates, knowledge about the HK was valuable when predicting streamflow.

The storage properties of a catchment provide valuable information about the residence time of the water in the catchment, and hence the temporal aspect of aquifer drainage. This information was therefore especially important when investigating the predictions relating to the timing and duration of Q95 low flow rates (Floriancic et al., 2016). Since Gore is located at the outlet of the catchment (and
thus effectively integrates the entire catchment), SS and SY contribute significantly to both predictions located at Gore.

In contrast, the SS and SY do not contribute significantly to the uncertainty for the predictions at McKellar Stream. This was because McKellar Stream is a spring-fed stream and therefore more directly related to the groundwater levels directly surrounding the stream, rather than the timing of the aquifer drainage (which is informed by SS and SY).

It was somewhat surprising that the HCOND (streambed conductance) does not contribute to the uncertainty. Lackey et al. (2015) among others, demonstrated that the streambed conductance plays a role when investigating stream depletion. In their model the stream depletion is influenced by a combination of HK, INCISN and HCOND. The fact that HCOND and INCISN do not contribute to uncertainty significantly in this study could be because the predictions used in this study were highly related to the aquifer flow system and thus, when all parameters were together, the contribution to uncertainty by HK, SS, and SY dominate over the contribution of HCOND and INCISN. It is expected that more local predictions may be more sensitive to these stream parameters, and this could be tested in future work.

6.1.2 Data Worth

6.1.2.1 The Worth of Observation Groups for the Low Flow Predictions

Overall, the groundwater level data (both periodic and telemetry data) observation groups reduce the uncertainty the most significantly for all the low flow predictions at Gore and the consecutive days below Q95 prediction at McKellar Stream. This was because of the long data record (up to 11.6 years) and large spatial distribution of observation wells (185 observation locations) contained in these datasets.

The groundwater telemetry data group (transient groundwater level data) reduces the uncertainty significantly more for the predictions at Gore. This was because the groundwater telemetry data greatly informs the SS and SY which play a larger role for the low flow predictions at Gore since these were integrating predictions. The catchment integrating nature of the predictions at Gore was also reflected by the fact that the spatially distributed groundwater observation wells reduce the uncertainty more significantly than the streamflow data (which is only available at 4 locations, Figure 6.2).

The surface water loss and gain observation group was the least informative for all low flow predictions at both Gore and McKellar Stream. This was because of the small amount of loss and gain observation locations (11 locations) and short record length (2-8 observations at each location) compared to the other observation groups.

The streamflow observation location Meadow Burn (Figure 6.2) is located close to the prediction location McKellar Stream, which explains why the streamflow observations data group contributed the most significantly to the uncertainty for the prediction days below Q95 and magnitude of stream depletion at McKellar Stream. In addition to the proximity of Meadow Burn to McKellar Stream, Meadow Burn is a spring-fed stream just as McKellar Stream, therefore it provides valuable information about the system state at McKellar Stream.

The transient groundwater level data (groundwater telemetry data) was more important for the prediction of the maximum duration of consecutive days below Q95 at McKellar Stream. It is likely that this result again reflects the importance of observations (transient groundwater level data) that provide information about the storage capacity (SS and SY) when predicting the Q95 low flow rates.

There was a vast amount of data present in the additional new wells observation group (1-year daily data of groundwater levels at 111 wells). Because of this, the largest reduction in uncertainty for all low flow predictions at both Gore and McKellar Stream was provided by the new additional wells observation group.
In terms of the low flow predictions studied here, there is some redundancy in parts of the observation dataset. This was evident in the discrepancies in the change in predictive uncertainty that occurs when it was assumed that a data group was subtracted from a complete dataset, compared to when it was assumed that there is no data and then a dataset was added. When the individual data groups were subtracted, the reduction in uncertainty remained high because of the vast amount of data that was available in the other observation groups.

6.1.2.2 The Spatial Pattern of Groundwater Level Data Worth for the Low Flow Predictions

The most uncertainty reducing observations for the low-flow predictions at Gore were scattered around the catchment area. This pattern was because the predictions at Gore were integrating predictions, which means that the predictions at this location are an integration of the entire catchment. Because of this, the observations throughout the catchment result in a reduction in uncertainty.

For the low-flow predictions at Gore the observations upstream in the north-east section of the mid-Mataura catchment reduce the uncertainty the most. This area coincides with the recharge zone, which means that there are larger fluctuations in groundwater. These larger fluctuations mean that the signal to noise ratio of the water levels was greater, and so provides clearer information than the smaller water level fluctuations towards Gore. This effect was especially large in this section of the study area because the aquifer is much thicker towards the north-east (Figure 6.1), where there is a greater ‘fill’ capacity within the aquifer, allowing larger groundwater level fluctuations in the recharge zone.

The most uncertainty reducing groundwater level observations for the low flow prediction at McKellar Stream were centred around the upstream section of McKellar Stream (Figure 5.8 B, D, and F). This pattern was because the predictions at this location were more discrete in nature. Discrete predictions are predictions that, because of the physical properties of the system at that prediction location, are informed more by data directly surrounding the prediction location. The McKellar Stream is spring-fed and thus receives water from the areas directly surrounding the stream, so observation providing information about the system state directly surrounding the prediction area reduce the uncertainty the most.

The spatial patterns in data worth were similar for the existing and additional groundwater level data. These patterns reflect the patterns for the discrete (low flow predictions at McKellar Stream), where the
observation directly surrounding the prediction location reduces the uncertainty the most, and integrating predictions (low flow predictions at Gore), where observations throughout the catchment reduce the uncertainty.

While the worth of additional groundwater level observations for the low flow predictions at Gore generally show a similar pattern to the existing observations, the analysis identified one significant additional groundwater level monitoring location, located in the area where all the sub streams converge before leaving the catchment; this possible future ‘converging stream’ groundwater level monitoring location reduces the uncertainty of the low flow predictions at Gore the most significantly.

It is expected that the spatial data worth patterns for integrating (observation throughout the catchment reduce the uncertainty) and discrete (observations directly surrounding the prediction location reduce the uncertainty the most) low flow predictions will show similar spatial data worth patterns in other catchments around the world.

6.1.2.3 Increased Spatial Data Worth of Groundwater Level Data
When exploring the worth of increasing spatial density of monitoring wells, it was shown that while less dense monitoring networks will result in a smaller reduction in uncertainty for spatially discrete predictions (e.g. the low flow predictions at McKellar Stream), the reduction in spatial monitoring density did not significantly impact the reliability of more integrating predictions (e.g. the low flow predictions at Gore). This was because of the vast amount of data available in the dataset (yearly data for the complete study period). When plotted on individual scales (Appendix A.6), it was clear that there was a smaller reduction in uncertainty when decreasing the spatial density of the monitoring wells.

6.1.2.4 Increased Temporal Data Worth of Groundwater Level Data
The comparison of predictive uncertainty that was achieved with increasing temporal monitoring frequencies indicated that there were diminishing returns for higher frequency monitoring data for the predictions examined. The analysis identified the importance of intra-annual variations when predicting low flows at Gore and McKellar, with a slight increase in uncertainty occurring when going from a daily, to weekly, to monthly monitoring frequencies, and then a sudden increase in uncertainty when monitoring occurs annually.

The reduction in uncertainty was uniformly high for the daily, weekly, monthly and annual monitoring frequencies when making the days below Q95 prediction. The reduction in uncertainty remained high for the days below Q95 prediction even when reducing the monitoring frequency, because of the vast amount of information available in the dataset.

6.1.2.5 Next Best Monitoring Locations for Additional Groundwater Level Data for Low Flow Predictions
If it was assumed that all existing monitoring networks (both groundwater level and stream flow) were retained, then the worth of each new additional possible measurement must consider the correlation of each new measurement with the existing monitoring network. When this was done, the pattern of the “next best measurement” alters from the spatial data worth pattern described in 6.1.2.2 The Spatial Pattern of Groundwater Level Data Worth for the Low Flow Predictions. This analysis showed that there was already a significant amount of data available to inform this prediction as the additional wells are located some distance away from the ‘best’ monitoring locations indicated by the largest dots (this was especially shown for the magnitude of stream depletion prediction at McKellar Stream, Figure 5.8 F). This emphasizes the importance of considering the existing dataset when developing a new monitoring scheme.

6.1.2.6 The Spatial Pattern of Existing Stream Flow Data Worth for the Low Flow Predictions
For all low flow predictions and locations, the streamflow data at Mataura (at the outlet, Figure 6.2) reduces the uncertainty the most (63% to 69% reduction in uncertainty). This was because it integrates the entire catchment area. After that the streamflow data at Waimea reduces the uncertainty the most for the predictions at Gore, this was because of both its long record length (5.1 years) and location
(Figure 6.2). The Waimea observation location provided information about the streamflow of the entire western branch of the river system of the catchment. After Mataura, Meadow Burn reduces the uncertainty the most for the low flow predictions at McKellar Stream, despite its short record length (0.6 years). This was because of its close proximity to McKellar Stream and because it is a spring-fed stream, just as McKellar. Waikaia is located far upstream in the north-east corner of the catchment (Figure 6.2), this explains why this observation location reduced the uncertainty the least for all predictions at both Gore and McKellar Stream.

Figure 6.2 Streamflow observation locations (green diamonds), additional new wells (black dots), prediction locations (red dots). Catchment outline shown in red, blue lines indicate streams.

6.1.2.7 The Impact of Model Simplifications on the Reliability of the Spatial Pattern of Data Worth Analyses

When using the homogeneous parameterisation, it appears that almost all of the new additional data would significantly reduce the uncertainty. This was because there were far less parameters (one parameter each for HK, SS, and SY) to be informed by the data when using homogeneous parameterisation, resulting in a very high contribution to uncertainty by most of the observations. Thus, the data worth results can be thought of as becoming “corrupted” by the lack spatial heterogeneity. This was in line with the findings of Fienen et al. (2010).

The impact of parameter simplification experiments showed that data worth analysis based on a grid-cell based parameterisation (Figure 5.12) were very similar to those using pilot-points (Figure 5.8). A distinct difference between the two simplification scenarios was that, the worth of the data was generally lower when using the grid-cell based parameterisation compared to when using the pilot-point based parameterisation. This was because there were many more uncertain parameters to be informed by the same amount of data when using the grid-cell based parameterisation, resulting in a smaller contribution to uncertainty per observation.

It is therefore suggested that, when performing a data worth study for low flow predictions, at least a pilot-point based spatial parameterisation should be adopted. The use of a pilot-point parameterisation scheme (distance between pilot-points 2 km) captures the primary spatial parameter variability, which the homogeneous parameterisation lacks. However, it is worth noting here that the computational time
associated with performing data worth uncertainty analyses was much higher with a grid-cell based parameterisation. A pilot-point based scheme should therefore perhaps be considered a favourable option.

6.2 Water Quality

6.2.1 The Role of Parameters in Uncertainty

6.2.1.1 Parameter Contribution to Uncertainty
There was a strong correlation between the hydraulic conductivity, denitrification and porosity parameters (HK, DEN, and PORO) and the predictive uncertainty of the nitrate concentration predictions in both surface and groundwater in areas within or adjacent to the denitrifying zone. The HK and PORO provide information about the velocity with which the particles were transported through the catchment, which provides information about the amount of time available for the denitrification process (DEN) to take place as groundwater travels through denitrifying zones within the aquifer. Thus, if these parameters were shown to significantly contribute to uncertainty for a specific location, it effectively shows the importance of the denitrification capacity of the catchment for that specific prediction.

If the prediction location was further away from the denitrification zone, then the recharge parameters (mRECH) contributed the most to the predictive uncertainty. This was because the nitrate source gets applied to the groundwater system through the recharge term in the groundwater model. Thus, if the denitrification does not play a role for a specific prediction location, the nitrate source (that gets applied through the mRECH) was important.

From the above data worth patterns, it can be derived that the proximity of a prediction location to a denitrification zone determines which parameters contribute the most to uncertainty.

6.2.1.2 Increase in Post-Calibration Uncertainty Contribution
In both Figure 5.2 and 5.13 it is evident that the post-calibration contribution to predictive uncertainty was larger than the pre-calibration contribution to predictive uncertainty for certain parameters. This means that the contribution of these parameters to the prediction uncertainty becomes larger after the model was calibrated using the existing dataset. The difference was relatively small (less than 0.1). This was also seen by Moore et al. (2011), where they explained that this can occur because of the calibration induced correlation between the estimated parameters, which is distinct from any natural correlation between parameters that may exist. This can be related to the necessary model simplifications of the real world, which can result in parameter combinations compensating for the simplifications during the calibration process, sometimes resulting in an increase in parameter and predictive uncertainty (Doherty and Simmons (2013)).

6.2.2 Data Worth

6.2.2.1 The Worth of Observation Groups for Nitrate Concentration Predictions
The analyses undertaken indicated that the relative contributions of different parameters and observation groups to reducing predictive uncertainty showed consistent patterns for both the surface water and groundwater prediction locations.

For the predictions closer to the denitrification areas, the observation groups that inform the HK, PORO, and DEN parameters reduce the uncertainty of the nitrate concentration predictions the most. These observations include: groundwater nitrate concentration, groundwater level, and surface water loss and gains.

Depending on the prediction location, the proximity of the observation location to the denitrification zone was significant. Where the prediction location is further from the denitrification zone, the data which provides information about the nitrate source concentration (e.g. groundwater and surface water
nitrate concentration data) was the most significant in terms of reducing predictive uncertainty. Prediction locations that were neither close nor significantly distant from the denitrification areas show that both data types were important (e.g. McKellar at Waimea, Figure 5.14 D).

The worth of the existing surface water concentration data observation group was generally low for all predictions, and this is most likely a result of the relatively small size of this data set (in total 39 observations). However, the analysis of the predictive uncertainty reduction based on the new additional surface water observation group, which is made up of surface water concentration observation in every model reach (in total 1165 observations) significantly reduces the predictive uncertainty. This was particularly the case for the prediction locations that were further away from the denitrification areas, again demonstrating the importance of concentration data for prediction location further away from the denitrification areas.

The additional new surface water streamflow was the most important for the surface water nitrate prediction Mataura at Gore (Figure 5.17 A). This was because the predictions located at Gore effectively integrate the entire catchment area, and therefore the vast amount of data that was available in this group (in total 1165 observations) significantly reduces the uncertainty for the surface water nitrate concentration prediction for the Mataura at Gore.

Interestingly, the additional new groundwater nitrate concentration data group i.e. from wells located in every 10th model cell, was never the most uncertainty reducing. This was because there were less observations in this group (a total of 111 observations) compared to the existing groundwater nitrates observation group, which comprises of a total of 124 nitrate concentration observation locations.

In contrast to the water quantity analyses, the difference between the data worth analyses undertaken by adding data to an empty dataset, and that undertaken by subtracting data from a complete calibration dataset, was more consistent for the water quality predictions. This was particularly so for those prediction locations further away from the denitrification zones. This result indicates that there is currently little redundancy in the dataset when predicting nitrate concentrations in areas further away from the denitrification areas.

**6.2.2.2 The Spatial Pattern of Data Worth for Nitrate Concentration Predictions**

The spatial patterns of data worth for the existing groundwater concentration data, the additional groundwater concentration data and the additional surface water concentration observations were very similar. In all three cases, these appear to depend on the proximity of the prediction location to the denitrifying areas.

For prediction locations close to the denitrifying areas, the observations downstream, close to the outlet of the catchment, were the most uncertainty reducing. This could be because these were integrating predictions, and thus the concentration at the outlet of the catchment will provide information about the system state at the prediction location.

For those predictions of a more spatially discrete nature, that were located further away from the denitrifying area (i.e. Meadow Burn at Mataura and N Well) the most uncertainty reducing observations were located directly surrounding the prediction location.

It is expected that the data worth patterns for nitrate concentration predictions in other catchments around the world will also depend as well on the proximity of the prediction location to the denitrifying areas.

**6.2.2.3 Next Best Monitoring Locations for Nitrate Concentration Predictions**

The patterns of next most important added observations were similar for both the additional groundwater nitrate concentration data and the surface water nitrate concentration data. There was again
a clear distinction between prediction locations close to the denitrification areas and further away. For the prediction locations close to the denitrification sites the next best observations were scattered through the catchment, with an emphasis on the denitrification areas (mid-western section of the catchment).

Expect for two discrete prediction locations (McKellar Stream at Mataura and Cooper’s Bore) for which the next most uncertainty reducing observations were centred around the prediction locations. The predictions at a greater distance from the denitrification areas (Meadow Burn and N Well) show that the next best observations were scattered around the prediction location.

As for the quantity data, these patterns of next best observations once again show the importance of considering the existing dataset, as was discussed in 6.1.2.3 Next Best Monitoring Locations for Low Flow Predictions.

6.3 Future Research
The study has identified a number of areas that could be explored in future work.

Firstly, to extend the assessment of data worth, the costs of acquiring data could be considered for the low flow predictions examined in this study. Wallis et al. (2014) demonstrated the importance of considering the costs when examining the data worth in the context of predicting travel times. Wallis et al. (2014) indicated that the most uncertainty reducing data might not necessarily be the most cost-effective option, and a greater number of cheaper but less informative data, may offer the greatest monitoring returns in terms of improving predictive reliability. It is therefore crucial to consider the costs of monitoring data when designing field monitoring programs.

Next to that, it is recommended to explore the worth of new additional stream flow observations for the stream depletion predictions at Gore and McKellar. The existing stream flow observations reduced the uncertainty the most for the days below Q95 and the magnitude of the stream depletion predictions at McKellar Stream. It would therefore be interesting and informative to see the spatial data worth pattern of the additional new streamflow data, and how this compares with the additional groundwater level data, given that one of the suspected reasons for a lower data worth of existing stream flow data was due to a paucity of measurements compared to the groundwater level data. This would also be important to consider when designing field monitoring programs in this region.

It is also recommended to explore in more detail why the streambed conductance (HCOND) does not contribute significantly to the uncertainty, while that would be expected when looking at the literature (e.g. Lackey et al., 2015). This would include a comparison of data worth for very localised stream depletion predictions, with the wider system based stream low flow prediction that have been examined in this study.

In this study, the effects of model parameter simplification on the water quality section of the study is not explored. In future research, it is therefore highly recommended to investigate the impact of having a steady state transport model versus a transient transport model and investigate the worth of having transient observation data. Next to that, it is recommended to investigate the impact of a 1-layer model versus a 3-layer model on the (spatial) data worth.

For the change in nitrate prediction the nitrate loading was doubled, in future research it is recommended to set more reasonable future nitrate levels after the land use change, this will lead to lower values in some areas and higher values in other compared to the situation after land-use change used in this study. Using this new scenario, the spatial worth of data when predicting the difference in nitrate concentration can be investigated in more detail.

And finally, it is recommended to investigate the worth of pre-processed data (e.g. physiographic zones). The physiographic zones (see section 2.2 Physiographic zones) were based on the existing dataset and provide information about the subsurface and the contaminant pathways. An interesting
study would be to quantify the worth of the physiographic zones when predicting the change in nitrate as a result of land-use changes, in this way it can be investigated if pre-processed data is worth it in the context of land-use change predictions.
7. Summary and Conclusion

For effective water resource management, a robust understanding of the system is necessary. In order to understand the system, managers need to make difficult decisions about what types of data to collect and where and when to collect it. Data worth methods can provide valuable support during this decision-making process. This master’s thesis aimed to optimize data collection efforts to support water and land use management, and specifically focused on: (i) the management of pumping-induced stream depletion impacts on stream low flow periods and (ii) the water quality impacts from increases in nitrate fluxes to the subsurface caused by land-use changes. Effective data collection was investigated by exploring the following questions:

Water Quantity questions:
- How well are the flow model parameters informed by the existing data? What is the role of parameters in uncertainty?
- How valuable is the existing data, and which type of additional data, collected where and when, will be the most valuable when predicting the number of days, and number of consecutive days, below a specified low stream flow rate (e.g. a Q95 flow rate), and what the pumping induced stream depletion rate?
- How do the spatial data worth patterns differ when the predicting impacts at different locations e.g. at Gore and McKellar Stream?
- For the predictions of the number of days below the Q95 flow rate and the magnitude of stream depletion rate: how is the reduction in uncertainty impacted when having a less dense monitoring network? How is the reduction in uncertainty impacted when decreasing the monitoring frequency?
- Are the data worth analysis results for the water quantity predictions impacted by model parameterisation simplifications? How are the final results impacted if a model uses a homogeneous, pilot-point, or grid-cell based parameterisation?

Water Quality questions:
- What is the role of the parameters in the uncertainty surrounding water quality predictions?
- How valuable is the existing data, and which type of data, collected at which location, will be the most valuable when predicting the change in nitrate concentration resulting from land use change? Is there a difference in the data worth results between the groundwater and surface water nitrate predictions?

To answer the questions the First Order Second Moment (FOSM) based data worth analysis method was employed. To implement this data worth method for the questions listed above a flow model (using the MODFLOW-NWT software) and a transport model (using MT3D-USGS) for the mid-Mataura catchment in Southland, New Zealand were used. The worth of the existing data as well as additional transient groundwater level data, groundwater nitrate concentration data, and surface water nitrate concentration data was calculated. The study was divided into a water quantity and water quality section.

The water quantity section focused the data worth analysis on predictions made at two locations: the catchment outlet at Gore, and the outlet of the spring-fed McKellar Stream. Three different predictions were made at these two locations: 1) the difference in the number of days below Q95 between the original model and a model with additional pumping wells. 2) the difference in the number of consecutive days below Q95 between the original model and a model with additional pumping wells. 3) the difference in the stream discharge flow rate between the original model and a model with additional pumping wells. For the water quantity predictions, the impacts of hydraulic parameter density scenarios were also investigated, with the following parameterisation options explored: i) distributed pilot-point parameters, ii) homogeneous parameters, and iii) grid-cell based parameters.
The water quality section focussed the data worth analysis on predicted nitrate concentration differences between the original transport model and a model with double the nitrate loading. The concentration differences were predicted at seven locations, 4 key surface water periphyton monitoring locations, and 3 key groundwater locations. The worth of both existing and additional potential monitoring data was investigated.

7.1 Water Quantity Conclusions
For the water quantity section of the study, it can be concluded that the hydraulic conductivity parameters were the best informed by the existing dataset and contribute the most to uncertainty for low flow predictions at both Gore and McKellar Stream. Next to that the results showed that data that provides information about the storage capacities of the catchment (i.e. long-term transient groundwater level data in the groundwater telemetry monitoring data) were most valuable for the predictions concerning the low stream flows (e.g. Q95 flows), this was because the storage capacity of the catchment is important in determining the timing of low flow periods.

It can also be concluded that the spatial data worth pattern was dependent on the prediction location. For Gore, the observations upstream in the north-west section of the mid-Mataura catchment were significant for reducing uncertainty of the low flow predictions, this was because the predictions at Gore effectively integrate the entire catchment area and were therefore sensitive to the long-term transient recharge trends in the catchment. The upper catchment, coincides with the recharge zone and where the aquifer is also thickest, such that groundwater level fluctuations are largest in this region, providing the clearest recharge trend information in the catchment.

In contrast, McKellar Stream is a spring-fed stream, and therefore its flows were most sensitive to groundwater levels immediately surrounding the springs. Because of this, the local data surrounding the upstream section of the McKellar Stream reduce the uncertainty the most.

From this can be derived that in general for integrating predictions (low flow predictions at Gore), concerning water quantity, the observations throughout the catchment reduce the uncertainty the most significantly, and that for discrete predictions (low flow predictions at McKellar Stream) the observations directly surrounding the prediction location reduce the uncertainty the most significantly.

The spatial data worth patterns do not differ when considering both existing and additional new data. The spatial diminishing return plots showed that the predictions at McKellar Stream had a larger reduction in uncertainty when having a less dense monitoring network, compared to the reduction in uncertainty for the predictions at Gore. From this can be concluded that the impact of having a less dense monitoring network was greater for discrete observations (e.g. spring-fed streams) as opposed to integrating predictions.

The temporal diminishing return plots demonstrated that there was a steady decrease in change in uncertainty when reducing the monitoring frequency from daily, to weekly, to monthly, followed by a bigger drop when monitoring annually. This indicates that the intra-annual variability is important when predicting pumping induced stream depletion, but that monitoring more frequent than monthly does not result in significant larger reduction in uncertainty. From this can be concluded that, when predicting pumping induced stream depletion, monthly monitoring is the preferred monitoring frequency.

The impact of spatial parameter simplification experiments showed that the spatial worth of the additional new data based on a grid-cell based parameterisation show similar patterns, in terms of data worth, as when using pilot-points. However, when using the homogeneous parameterisation, the data worth results became corrupted by the lack of spatial variability available in the parameterisation. From this can be concluded that a certain degree of spatial variability is needed (e.g. pilot-points) in order to identify the spatial worth of data when predicting pumping induced stream depletion, but that a more detailed parameterisation (e.g. grid-cell based) does not provide significantly more information about the spatial data worth patterns.
It can thus be concluded that spatial variability is needed when performing a data worth study (as was shown by Fienen et al. 2010). Since, the data worth analysis using the grid-cell based parameterisation was much more computational intense than when using the pilot-point based parameterisation and the data worth analysis using the grid-cell based parameterisation does not provide significant more information it can be concluded that the pilot-point based parameterisation should be considered the favourable option.

7.2 Water Quality Conclusions
In the water quality section, it was shown that there was a coincidence of importance of the hydraulic conductivity, porosity, and denitrification rate parameters in areas within or near denitrifying zones. This was because the hydraulic conductivity and porosity parameters provide information about the velocity of the groundwater, which provides information about the amount of time available for denitrification to take place. Thus, when it was shown that these three parameters contribute to the uncertainty for a specific prediction location, it effectively means that the denitrification was important for that prediction location. At other prediction locations, more removed from denitrifying zones, it was shown that the source term, which was incorporated in the data worth analysis recharge concentration, was the most important.

The spatial data worth patterns showed that, there was not a distinct difference between surface water and groundwater prediction locations, but that both surface and groundwater spatial data worth patterns depend on the distance between the prediction location and the area where denitrification takes place. If the prediction location was further away from the denitrifying area, observations around the prediction location itself reduce the uncertainty the most. From this can be concluded that, when predicting change in nitrate concentrations as a result of land-use change, the spatial data worth pattern greatly depends on the proximity of the prediction location to the denitrifying area.

7.3 Future Studies
Future studies that aim to develop a monitoring network for low flow predictions should consider that when predicting low flows, it should be determined if the prediction of interest is an integrating or a discrete prediction, since this will determine where the most uncertainty reducing observations would be. If it is a discrete prediction the data surrounding the prediction location will result in the largest reduction in uncertainty, and if it is an integrating predictions the observations throughout the catchment will reduce the uncertainty the most.

Next to that in future studies it should be taken into account that, when predicting low flows, the spatial heterogeneity of the system should be represented, but that a more detailed parameterisation than pilot-points (e.g. grid-cell based parameterisation), does not provide a significant amount of extra information and is due to the long computational time not recommended. Pilot-point based parameterisation should therefore be considered the favourable option.

Also, in future studies should be taken into account that the location of the denitrifying areas, and the proximity of the prediction locations to these areas, will greatly determine data worth patterns.
References


- Bayes, T. (1763). A letter from the late Reverend Mr. Thomas Bayes, FRS to John Canton, MA and FRS. Philosophical Transactions (1683-1775), 53, 269-271.


Appendix

A.1 Covariance structures used to make the covariance matrices used in the uncertainty analysis.

STRUCTURE str_mRECH
NUGGET 0.0
TRANSFORM log
NUMVARIOGRAM 1
VARIOGRAM exp_2k 0.01
END STRUCTURE

STRUCTURE str_HK
NUGGET 0.05
TRANSFORM log
NUMVARIOGRAM 1
VARIOGRAM exp_2k 0.64
END STRUCTURE

STRUCTURE str_VK1
NUGGET 0.0
TRANSFORM log
NUMVARIOGRAM 1
VARIOGRAM exp_2k 0.3
END STRUCTURE

STRUCTURE str_SS
NUGGET 0.0
TRANSFORM log
NUMVARIOGRAM 1
VARIOGRAM exp_2k 0.3
END STRUCTURE

STRUCTURE str_Sy
NUGGET 0.0
TRANSFORM log
MEAN -1.6
NUMVARIOGRAM 1
VARIOGRAM exp_2k 0.3
END STRUCTURE

STRUCTURE str_poro
NUGGET 0.0
TRANSFORM log
MEAN -1.7
NUMVARIOGRAM 1
VARIOGRAM exp_2k 0.4
END STRUCTURE

STRUCTURE den
NUGGET 0.0
TRANSFORM log
MEAN -1.7
NUMVARIOGRAM 1
VARIOGRAM exp_2k 0.2
END STRUCTURE

VARIOGRAM exp_2k
VARTYPE 2
BEARING 0.0
A 6000.0
ANISOTROPY 1.0
END VARIOGRAM
A.2. Python script that calculates the data worth, for both subtraction and addition, and it calculates the order of the next most important added observation for all water quality predictions.

### pyEMU transport

In[1]:

```python
get_ipython().magic('matplotlib inline')
import os
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import shutil
import flopy
import pyemu
import shapefile
import copy
```

```python
# ## Setting forcasts
# In[2]:

forecasts = ['diff_n_cooper', 'diff_n_jacobs', 'diff_n_wel_3', 'diff_n_mck_wai',
             'diff_n_mea_rou', 'diff_n_wai_mat', 'diff_n_mat_gor']
```

```python
# ### Calculating the Schur compliment
# In[3]:

sc = pyemu.Schur(jco="original_transport.jco",forecasts=forecasts,verbose=True,parcov="transport.prior.jcb")
sc_groups = pyemu.Schur(jco="transport_groups_original.jco",forecasts=forecasts,verbose=True,parcov="transport.prior.jcb")
sc_new = pyemu.Schur(jco="transport_new_data.jco",forecasts=forecasts,verbose=True,parcov="transport.prior.jcb")
sc_groups_new = pyemu.Schur(jco="transport_groups_new_data.jco",forecasts=forecasts,verbose=True,parcov="transport.prior.jcb")
```

```python
# ### Calculating parameter contribution to uncertainty
# In[4]:

con = sc.get_par_group_contribution(include_prior_results=True)
con_good = (abs(con-con.loc["base",:]))/con.loc["base",:]
cont_good = con_good.loc["den":"poro",:]
```

```python
# In[5]:

plt.rcParams.update(plt.rcParamsDefault)
con_good.plot(kind="bar", subplots=True, figsize=(7,20), color="g", fontsize = 11,
sharex=False, legend=False)
plt.tight_layout()
plt.savefig("parameter contribution to uncertainty")
plt.show()
```

```python
# ### Calculating the change in uncertainty after observation groups are added (predunc5 addition)
# In[6]:

df_add = sc.get_added_obs_group_importance()
df_add_groups = sc_groups.get_added_obs_group_importance()
df_add_new = sc_new.get_added_obs_group_importance()
df_add_groups_new = sc_groups_new.get_added_obs_group_importance()
df_add.to_csv(os.path.join("analyses_pyemu","transport_original_addition.txt"),sep=' ')
df_add_groups.to_csv(os.path.join("analyses_pyemu","transport_original_addition.txt"),sep=' ')
df_add_new.to_csv(os.path.join("analyses_pyemu","transport_new_data_addition.txt"),sep=' ')
df_add_groups_new.to_csv(os.path.join("analyses_pyemu","transport_groups_new_data_addition.txt"),sep=' ')
```
# Calculating change in uncertainty after addition

```python
# In[8]:

df_add_good = (abs(df_add - df_add.loc["base",:]))/df_add.loc["base",:]
df_add_good.to_csv(os.path.join("analyses_pyemu","transport_good_addition_phizzies.txt"),sep=';')
df_add_groups_good = (abs(df_add_groups - df_add_groups.loc["base",:]))/df_add_groups.loc["base",:]
df_add_groups_good.to_csv(os.path.join("analyses_pyemu","transport_good_addition_groups.txt"),sep=';')
df_add_new_good = (abs(df_add_new - df_add_new.loc["base",:]))/df_add_new.loc["base",:]
df_add_new_good = df_add_new_good.loc["add_sw":"sw_strmflow"]
df_add_new_good.to_csv(os.path.join("analyses_pyemu","transport_good_addition_new.txt"),sep=';')
df_add_good = df_add

# Calculating the change in uncertainty after observation groups are subtraction (predunc5 subtract)

# In[9]:

df_subt = sc.get_removed_obs_group_importance()
df_subt_groups = sc_groups.get_removed_obs_group_importance()
df_subt_new = sc_new.get_removed_obs_group_importance()
df_subt_groups_new = sc_groups_new.get_removed_obs_group_importance()
df_subt.to_csv(os.path.join("analyses_pyemu","transport_original_subtract.txt"),sep=';')
df_subt_groups.to_csv(os.path.join("analyses_pyemu","transport_groups_original_subtract.txt"),sep=';')
df_subt_new.to_csv(os.path.join("analyses_pyemu","transport_new_data_subtract.txt"),sep=';')
df_subt_groups_new.to_csv(os.path.join("analyses_pyemu","transport_groups_new_data_subtract.txt"),sep=';')

df_subt_good = (abs(df_subt - df_subt.loc["base",:]))/df_add.loc["base",:]
df_subt_good = df_subt_good.loc["g1_tr":"sw_strmflow"]
df_subt_good.to_csv(os.path.join("analyses_pyemu","transport_good_subtraction_phizzies.txt"),sep=';')
df_subt_groups_good = (abs(df_subt_groups - df_subt_groups.loc["base",:]))/df_add_groups.loc["base",:]
df_subt_groups_good.to_csv(os.path.join("analyses_pyemu","transport_good_subtraction_groups.txt"),sep=';')
df_subt_new_good = (abs(df_subt_new - df_subt_new.loc["base",:]))/df_add_new.loc["base",:]
df_subt_new_good = df_subt_new_good.loc["add_sw":"sw_strmflow"]
df_subt_new_good.to_csv(os.path.join("analyses_pyemu","transport_good_subtraction_new.txt"),sep=';')
df_subt_groups_new_good = (abs(df_subt_groups_new - df_subt_groups_new.loc["base",:]))/df_add_groups_new.loc["base",:]
df_subt_groups_new_good.to_csv(os.path.join("analyses_pyemu","transport_good_subtraction_new_groups.txt"),sep=';')

# Visualizing results

# In[11]:

plt.rcParams.update(plt.rcParamsDefault)
ax = df_subt_good.plot(kind="bar", subplots=True, figsize=(7,60), color="g", fontsize=11, sharex=False, legend=False, width=0.5, align="edge")
df_add_good.plot(ax=ax, kind="bar", subplots=True, figsize=(7,60), color="b", fontsize=11, sharex=False, legend=False, width=0.5, align="edge")
plt.tight_layout()
plt.savefig("Addition_subtraction_original")
plt.show()
```

# In[]:
ax = df_subt_new_good.plot(kind="bar", subplots=True, figsize=(7,60), color="g", fontsize=11, sharex=False, legend=False, width=0.5, align='edge')
df_add_new_good.plot(ax=ax, kind="bar", subplots=True, figsize=(7,60), color="b", fontsize=11, sharex=False, legend=False, width=0.5, align='edge')
plt.tight_layout()
plt.savefig("Addition_subtraction_new_data")
plt.show()

# ### Calculating next most important added observation
# In[ ]:
# Making the 'base list' which contains all the existing observations
# and the 'obslist_dict' which contains all the new potential observations
 obslist_dict = sc_groups_new.obs_group_importance()
obslist_dict = {k: obslist_dict[k] for k in obslist_dict if "add_well" in k}
for k, lst in obslist_dict1.items():
    if not "add_well" in k and not "baseflow" in k and not "add_sw" in k:
        base_obslist.extend(lst)

# In[ ]:
next_most_diff_n_cooper =
sc_groups_new.next_most_important_added_obs(forecast="diff_n_cooper", obslist_dict=obslist_dict,
base_obslist=base_obslist, niter=10)
next_most_diff_n_cooper.to_csv(os.path.join("analyses_pyemu","next_most_important_diff_n_cooper.txt"),sep="")

# In[ ]:
next_most_diff_n_well_2 =
sc_groups_new.next_most_important_added_obs(forecast="diff_n_well_3", obslist_dict=obslist_dict,
base_obslist=base_obslist, niter=10)
next_most_diff_n_well_2.to_csv(os.path.join("analyses_pyemu","next_most_important_diff_n_well_3.txt"),sep="")

# In[ ]:
next_most_diff_n_mat_gor =
sc_groups_new.next_most_important_added_obs(forecast="diff_n_mat_gor", obslist_dict=obslist_dict,
base_obslist=base_obslist, niter=10)
next_most_diff_n_mat_gor.to_csv(os.path.join("analyses_pyemu","next_most_important_diff_n_mat_gor.txt"),sep="")

# In[ ]:
next_most_diff_n_mea_rou =
sc_new.next_most_important_added_obs(forecast="diff_n_mea_rou", obslist_dict=obslist_dict,
base_obslist=base_obslist, niter=10)
next_most_diff_n_mea_rou.to_csv(os.path.join("analyses_pyemu","next_most_important_diff_n_mea_rou.txt"),sep="")

# In[ ]:
next_most_diff_n_jacobs =
sc_new.next_most_important_added_obs(forecast="diff_n_jacobs", obslist_dict=obslist_dict,
base_obslist=base_obslist, niter=10)
next_most_diff_n_jacobs.to_csv(os.path.join("analyses_pyemu","next_most_important_diff_n_jacobs.txt"),sep="")

# In[ ]:
next_most_diff_n_wai_mat =
sc_new.next_most_important_added_obs(forecast="diff_n_wai_mat", obslist_dict=obslist_dict,
base_obslist=base_obslist, niter=10)
next_most_diff_n_wai_mat.to_csv(os.path.join("analyses_pyemu","next_most_important_diff_n_wai_mat.txt"),sep="")

# In[ ]:
next_most_diff_n_mck_wai = 
sc_new.next_most_important_added_obs(forecast="diff_n_mck_wai",obslist_dict=obslist_dict,
base_obslist=base_obslist, niter=10)
next_most_diff_n_mck_wai.to_csv(os.path.join("analyses_pyemu","next_most_important_diff_n_mck _wai_rou.txt"),sep=' ')
A.3. Proportional increase in uncertainty after the subtraction of existing groundwater level data for all the predictions: A) Difference in days below Q95 at Gore, B) Difference in days below Q95 at McKellar Stream, C) Magnitude of stream depletion at Gore, D) Magnitude of stream depletion at McKellar Stream. The colours are on a scale of 0 (blue) to 1 (red) and are the same for all figures. The dots show the groundwater level observation locations and the sizes of the dots are proportional to the percentage decrease in uncertainty and are prediction specific. The black dots with white circles around them are the additional wells and the red dots are the prediction locations.
A.4 Proportional increase in uncertainty after the subtraction of existing groundwater telemetry data for all the predictions: A) Difference in days below Q95 at Gore, B) Difference in days below Q95 at McKellar Stream, C) Magnitude of stream depletion at Gore, D) Magnitude of stream depletion at McKellar Stream. The colours are on a scale of 0 (blue) to 1 (red) and are the same for all figures. The dots show the groundwater level observation locations and the sizes of the dots are proportional to the percentage decrease in uncertainty and are prediction specific. The black dots with white circles around them are the additional wells and the red dots are the prediction locations.
A.5, Proportional increase in uncertainty after the subtraction of the additional new groundwater telemetry data for all the predictions: A) Difference in days below Q95 at Gore, B) Difference in days below Q95 at McKellar Stream, C) Magnitude of stream depletion at Gore, D) Magnitude of stream depletion at McKellar Stream. The colours are on a scale of 0 (blue) to 1 (red) and are the same for all figures. The dots show the groundwater level observation locations and the sizes of the dots are proportional to the percentage decrease in uncertainty and are prediction specific. The black dots with white circles around them are the additional wells and the red dots are the prediction locations.
A.6. Spatial diminishing return plots. Proportional reduction in uncertainty after adding daily telemetry data for the complete model time (15 years) in every 10th, 20th, and 30th cells. A) Difference in days below Q95 at Gore, B) Difference in days below Q95 at McKellar Stream, C) Magnitude of stream depletion at Gore, D) Magnitude of stream depletion at McKellar Stream. Y-axis is prediction and location specific and should therefore not be compared directly, relative patterns can be compared.
A.7. Temporal diminishing return plots. Proportional reduction in uncertainty after adding groundwater telemetry data in every tenth cell with daily, weekly, monthly or annual data for the complete study period. A) Difference in days below Q95 at Gore, B) Difference in days below Q95 at McKellar Stream, C) Magnitude of stream depletion at Gore, D) Magnitude of stream depletion at McKellar Stream. Y-axis is prediction and location specific and should therefore not be compared directly, relative patterns can be compared.
Glossary

Calibration  The process of matching model outputs to observation data through the adjustment of parameters (Beven, 2011).

Catchment  An area where all the precipitation drains through one outlet (Skinner et al. 2000).

Jacobian Matrix  Also commonly referred to as the sensitivity matrix. It is an m by n matrix, in which m are the model outputs and n are the model parameters. The elements of the matrix provide information about the sensitivity of the model parameters on the model outputs (Doherty et al., 2015).

Kriging  A spatial interpolation technique that derives the value for an unmeasured location by weighing the surrounding measurements (Cressie, 1990).

Structural (epistemic) noise  Noise, or uncertainty that is inherent to the system due to the imperfect knowledge or understanding of the system.